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Introduction to Quantum Backflow

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Abstract

La tesi si propone di analizzare il fenomeno del *backflow* quantistico per particelle vincolate a muoversi in una direzione. Dapprima si affronterà lo studio nel caso di particelle non interagenti e successivamente si generalizzeranno i risultati ottenuti nel caso interagente sotto l'effetto di potenziali a corto raggio.

The aim of the thesis is to analyse the phenomenon of quantum *backflow* for particles traveling on a straight line. First of all, the phenomenon will be studied in a non-interacting framework and then the results will be generalized for the interacting scenario, where a short-range potential is applied.

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Introduction

Backflow is an exotic quantum-mechanical phenomenon where for a particle with right-pointing momentum the flux of probability across a reference point may be left-pointed.
In detail, we consider non-relativistic particles which travel on a straight line. In *quantum mechanics*, we describe the state of this particles at a given instant of time with a *wave-function* $\psi : \mathbb{R} \to \mathbb{C}$ such that $|\psi(x)|^2$ represents the density probability function of finding the particle in region of space $\mathbb{R}$. The time-evolution of such wave-functions $\psi(t)$ is given by the *Schrödinger equation*

$$i\partial_t \psi(t) = H\psi(t)\,, \tag{1}$$

where H is the *Hamiltonian* which describes the interactions of a particle and where we set all the parameters and physical constants equal to 1. Furthermore, we restrict us to consider particles that "travel to the right". This means that a wave-function has only positive components for the momentum. Stated differently, the Fourier transform of this wave-function in *momentum space*

$$\widehat{\psi}(p,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ipx} \psi(x,t)\,\mathrm{d}x \tag{2}$$

is supported only for $p > 0$. Such wave-functions will be called *right-movers*.
In this scenario, one might classically think that the density probability function must flow to right for all times and everywhere in space. Hence the probability of finding the particle on the right of a given reference point might seem to be increasing with time. Against expectations, in some cases this probability decreases with time. This is what it is meant for *quantum backflow*.
The scope of this dissertation, is to report and discuss the main results regarding the strength and all other fundamental properties of backflow in two different scenarios: *non-interacting* and *interacting* case.
For *free particles*, we will prove that the amount of probability which can "flow back" through a reference point in a given interval of time is always less than suitable *backflow constant* λ which has been estimated to be $\lambda \approx 0.038452$. In particular it will turn out that the backflow constant corresponds to the infimum of the spectrum of a suitable bounded and self-adjointed operator, called backflow operator. We will also report numerical estimation of the backflow constant λ using the *power method*. We

will also ~~investigate~~ the spatial extension of backflow ~~by considering~~ spatial integrals of the density current $j_\psi(x) = i/2(\psi(x)\partial_x\psi^*(x) - \psi^*(x)\partial_x\psi(x))$. In detail, we will prove that there exists a constant $\beta_0(f)$ such that

$$\int_{-\infty}^{\infty} f(x) j_\psi(x)\,\mathrm{d}x \geq \beta_0(f) > -\infty \tag{3}$$

for all normalized right-moving wave functions and for all positive averaging functions $f \geq 0$.
In the *interacting scenario*, We will investigate the presence of backflow for particles which scatters against some potential wall V. In this scenario, complications arises since the presence of a potential V implies the splitting of the incident wave-function into a transmitted and a reflected wave which travel in opposite direction. This makes the concept of "right-moving" particles less clear. Hence we will introduce *asymptotics* right-movers as those wave-functions that far away in the past, and far away from the potential wall V, behaves like free and right-moving wave-functions. If we consider a non-interacting right-mover ϕ, it might be seen as the incoming asymptote of an interacting state ψ. The link between the two wave-functions is given by the *Møller operator* Ω_V of the Hamiltonian with the potential V ~~as~~ $\psi = \Omega_V\phi$. ~~Once we reminded the fundamental concept~~ about scattering theory, we generalize the result ~~in~~ (3) ~~in~~ scattering situations. Hence we will study lower bounds for the average

$$\int_{-\infty}^{\infty} f(x) j_{\Omega_V\psi}(x)\,\mathrm{d}x \tag{4}$$

for a generic normalized right-mover ψ and for a positive function $f \geq 0$. Although reflection process can amplify backflow, we will prove that there exists, for all short range potential V and for all positive smearing functions $f \geq 0$, a constant $\beta_V(f) > -\infty$ such that

$$\int_{-\infty}^{\infty} f(x) j_{\Omega_V\psi}(x)\,\mathrm{d}x \geq \beta_V(f) \tag{5}$$

for all normalized right-mover ψ.

~~A synopsis of the thesis is the following:~~
In the first chapter, it will be presented an overview of the main mathematical notions needed in order to set the discussion on quantum mechanics and backflow. The main topics will be *Hilbert spaces*, *operators* and their *spectrum*, *Schwartz test-functions*, *Fourier transform* as well as the basic concepts of quantum mechanics with particular attention to the *interaction picture* in scattering scenarios and *Møller operators*.
In the second chapter, it will be discussed the backflow effect in non-interacting

scenario. First of all, we will begin with an historical overview on the results obtained across the years regarding quantum backflow; from first theoretical formulations, until the most recent analytical and numerical results. Then we introduce the problem of backflow for free-particle. We will define rigorously the concept of *right-mover* and give some examples of wave-functions in which backflow occurs. Then, we will search a lower bound for the flux of probability across a reference point in a given time interval. To do this, we must reformulate the problem as the search for an infimum of the spectrum of an operator called *backflow operator*. We will prove that such a lower bound exists and hence that the flux of probability across the reference point is always greater than $-\lambda$, where $\lambda \in (0,1)$ is the *backflow constant*. At the end of the chapter, numerical methods will be presented in order to estimate λ. In particular, using the *power method* we will evaluate a good approximation for the backflow constant of $\lambda \approx 0.038452$.
The third chapter is divided in two main section. In the first section, ~~it will be discussed~~ the spatial extension of backflow for normalized right-movers at a given instant of time. It will be proved that the average of the density current for a right-moving state, as in (3), is bounded from below with by a constant $\beta_0(f) \in (-\infty, 0)$. The second section will be dedicated to the analysis of backflow in scattering theory. First, the problem of backflow will be reformulated introducing the concept of *asymptotic* right-moving wave-functions. Then, we will study the existence of a negative lower bound for the average current, as in (5). To do so, the infimum of the spectrum of an unbounded operator, called *asymptotic current operator* will be searched. At the end, we will prove that backflow can occur also in scattering scenarios and that the average current is always bigger than a suitable constant $\beta_V(f)$ determined by the potential V and the positive smearing functions $f \geq 0$.

Chapter 1

Mathematical Tools

The aim of the first chapter is to introduce the theoretical set-up needed for our investigations. Here, we will outline the main mathematical tools and theorems that will be used in the study of quantum backflow. First of all, we will sum up the basic concepts of Hilbert spaces and the linear operators living on it. The second section will be entirely devoted to the introduction of the Fourier transform and of its properties which are essential in the study of kinematic aspects of particles. Last, we will focus on quantum mechanics summarizing the Schrödinger equation and the concept of observable as well as its connection with linear operators.

1.1 Hilbert Spaces and Operators

In quantum mechanics a wave function is a complex valued map ϕ whose square of absolute value $|\phi(x)|^2$ represents the distribution probability of finding the particle somewhere in the physical space. Generally, those functions are thought as elements of a particular vector space called Hilbert space. A complete definition of ~~this~~ important ~~concept~~ will be given in ~~the following~~ section.

First of all, we introduce a class of vector spaces in which we could define the "length" of a vector or the "distance" between two different vectors. Hence we have

1.1.1 Definition (Normed vector space). *Let V be a vector space in complex field. V is called normed space if there exists a map $\|\cdot\| : V \to \mathbb{R}$ such that:*

(a) $\|v\| \geq 0 \; \forall v \in V$, *and* $\|v\| = 0$ *if and only if* $v = 0$

(b) $\|\alpha v\| = |\alpha| \|v\| \;\; \forall \alpha \in \mathbb{C}, \; \forall v \in V$

(c) $\|v + w\| \leq \|v\| + \|w\| \; \forall v, w \in V$

and this map $\|\cdot\|$ is called norm of the space V.

1.1.2 Example. Consider the vector space $\mathbb{C}^n$ with the norm defined by $||z|| = \left[\sum_{i=1}^{n} |z_i|^2\right]^{\frac{1}{2}}$, where $z = (z_1, \dots, z_n) \in \mathbb{C}^n$. This is a normed space.

The definition of norm naturally introduce a concept of convergence in such vector space. In fact, we can define that a certain sequence $\{v_n\} \in V$ converges to a vector $v \in V$ if $\lim_{n\to\infty} \|v_n - v\| = 0$.
A well-known fact ~~from theory on~~ $\cancel{\mathbb{R}^n}$ is that convergent sequences $\{v_n\}_{n\in\mathbb{N}}$ in a normed space V satisfy the *Cauchy property* (see [1, Chap. 2]):

1.1.3 Definition (Cauchy sequences). *A sequence $\{v_n\}_{n\in\mathbb{N}}$ in a normed space V is called a Cauchy sequence if, for any $\varepsilon > 0$, there exists $N_\varepsilon \in \mathbb{R}$ such that $\|v_n - v_m\| < \varepsilon$ whenever $n, m > N_\varepsilon$.*

Now, we introduce the concept of *complete normed space.*

1.1.4 Definition (Banach spaces). *A normed space is called a Banach space if it is complete, i.e. if any Cauchy sequence inside the space converges to a point of the space.*

Now, we want to identify Hilbert spaces. In this new class of vector spaces we will be able to define the fundamental concept of scalar product.

1.1.5 Definition (Hilbert space). *Let $\mathcal{H}$ be a vector space over the complex field. $\mathcal{H}$ is a Hilbert space if there exists a map $(\cdot|\cdot) : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ (called scalar product) such that:*

(a) $(w|\alpha v_1 + \beta v_2) = \alpha(w|v_1) + \beta(w|v_2)\ \forall w, v_1, v_2 \in \mathcal{H},\ \forall \alpha, \beta \in \mathbb{C}$

(b) $(w|v) = \overline{(v|w)}\ \forall v, w \in \mathcal{H}$

(c) $(v|v) \geq 0\ \forall v \in \mathcal{H}$ *and* $(v|v) = 0$ *if and only if* $v = 0$

and if $\mathcal{H}$ is complete with the norm defined by $\sqrt{(\cdot|\cdot)}$.

1.1.6 Example. **(a)** $\mathbb{C}^n$ with the inner product $(u|v) := \sum_{i=1}^{n} \overline{u_i} v_i$, where $u = (u_1, ..., u_n)$, $v = (v_1, ..., v_n)$, is a Hilbert space.

(b) Consider the set

$$L := \left\{ f : \mathbb{R}^n \to \mathbb{C} \;\middle|\; \int_{\mathbb{R}^n} |f(x)|^2 \, \mathrm{d}^n x < \infty \right\} \tag{1.1}$$

and the equivalence class $[f]$ of a function $f \in L$:

$$[f] = \{g \in L \mid f = g \text{ almost everywhere}\}. \tag{1.2}$$

Then, we define the space $L^2(\mathbb{R}^n)$ as

$$L^2(\mathbb{R}^n) = \{[f] \mid f \in L\}. \tag{1.3}$$

$L^2(\mathbb{R}^n)$ is a Hilbert space with the scalar product defined by:

$$([f]|[g]) = \int_{\mathbb{R}^n} \overline{f(x)} g(x) \, \mathrm{d}^n x. \tag{1.4}$$

This space play a key role in quantum mechanics. In fact each wave function ϕ is considered as ~~an~~ element of this space ~~such~~ $\int_{\mathbb{R}^n} |\phi(x)|^2 \, \mathrm{d}^n x = 1$.[1]

Now we enunciate some notable definitions and results concerning the linear operators on normed and Hilbert spaces.

1.1.7 Definition. *Let V and V' be normed spaces. A linear map $T : D(T) \to V'$, where $D(T) \subseteq V$ is a subspace of V, is called a* ***linear operator****. Furthermore,*

(a) *if $D(T)$ is dense in V, T is called a* ***dense*** *operator*[2].

(b) *The set $\{Tv \mid v \in D(T)\}$ it is called* ***Range*** *of the operator T and it isindicated with the symbol $Ran(A)$.*

(c) *The set $\{v \in D(T) \mid Tv = 0\}$ it is called* ***Kernel*** *of the operator T and it is indicated with the symbol $Ker(A)$.*

(d) *T is a* ***closed*** *operator if its graph $G(T) := \{(v, Tv) \in V \times V' \mid v \in D(T)\}$ is a closed set. Instead T is a* ***closable*** *operator if there exists a closed extension of T (called $\overline{T}$).*

(e) *An operator $T : V \to V'$ is* ***bounded*** *if $\exists k \in (0, +\infty)$ such that*

$$\|Tv\| \leq k\|v\| \; \forall v \in V \tag{1.5}$$

or equivalently,

$$\|T\| := \sup_{\|v\|=1} \|Tv\| < +\infty \tag{1.6}$$

We represent the set of linear operators from V to V' with the symbol $\mathcal{L}(V, V')$ while bounded operators are indicated with $\mathcal{B}(V, V')$.

1.1.8 Observation. The basic property of bounded operators is that for any bounded subset of the domain V its image remains bounded. Furthermore, we prove that $\mathcal{B}(V)$ is also a normed space with the definition of norm given in Eq. (1.6).

[1] Hereafter, we shall write f instead of $[f]$.

[2] $D(T)$ is dense in V when for all $v \in V$ there exists a sequence $\{v_n\} \in D(T)$ converging to v.

1.1.9 Example. Consider the Hilbert space $L^2(\mathbb{R})$ and the derivative operator $P := -i\partial_x$ (called the *momentum* operator). P could not be defined for all the elements in $L^2(\mathbb{R})$. But it is well defined in the space of test-functions $C_0^\infty(\mathbb{R})$, which is a ~~closed~~ subspace of $L^2(\mathbb{R})$. Other examples of dense operators in $L^2(\mathbb{R})$ are the multiplication operator $X := x$ (called *position* operator) and $P^2 := -\partial_x^2$. All these operators will be investigated more in detail in the third part of the chapter.

1.1.10 Theorem. *Let be V and V' two normed space and $T : V \to V'$ a linear operator. Then the following statements are equivalent:*

(a) $T \in \mathcal{B}(V, V')$

(b) T *is continuous,*

(c) T *is continuous in* 0.

A proof of this theorem could be found in [1, Th. 2.43].

Another fundamental concept is that of *adjoint operator*. It is common to have to deal with the scalar product of a vector and the image of another vector under a linear operator. Take for example a linear operator $T : D(T) \to \mathcal{H}'$ and consider the scalar product:

$$(w|Tv) \text{ with } v \in D(T) \subseteq \mathcal{H},\ w \in \mathcal{H}'. \tag{1.7}$$

We ~~want to ask ourself~~ if there exists a particular operator T^* defined in some subspace $D(T^*)$ such that

$$(T^*w|v)\ \forall w \in D(T^*), v \in D(T) \tag{1.8}$$

More generally, we may ~~think about the first scalar product~~ as a linear functional $f_T : D(T) \to \mathbb{C}$ ~~which map~~ $v \mapsto f_T(v) := (w|Tv)$ and we ask whether there exists a particular vector w_f which *represents* our functional, i.e. $f_T(v) = (w^*|v)$. Here w^* has the same role of T^*w in the previous equation. In order to investigate ω existence:

1.1.11 Proposition (Existence of adjoint operator). *If $\mathcal{H}$ and $\mathcal{H}'$ are Hilbert spaces and $T \in \mathcal{B}(\mathcal{H}, \mathcal{H}')$, then there exists a unique adjoint operator $T^* \in \mathcal{B}(\mathcal{H}', \mathcal{H})$ such that*

$$(w|Tv) = (T^*w|v)\ \forall w \in \mathcal{H}',\ \forall v \in \mathcal{H}. \tag{1.9}$$

The existence of T^* is a consequence of the *Riesz's representation theorem* and a complete proof of the equivalence and of the other points above could be found on [1, Ch. 2-3].

Now, we classify different types of bounded operators.

1.1.12 Definition. *Let $\mathcal{H}$ and $\mathcal{H}'$ be Hilbert spaces.*

(a) *$T \in \mathcal{B}(\mathcal{H})$ is* ***self-adjoint*** *if $T = T^*$.*

(b) *$T \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ is* ***isometric*** *if $(Tv|Tw) = (v|w)$ for all $v, w \in \mathcal{H}$, or equivalently if $T \in \mathcal{B}(\mathcal{H}, \mathcal{H}')$ and $T^*T = \mathbb{I}_{\mathcal{H}}$.*

(c) *$T \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ is* ***unitary*** *if it is isometric and surjective , or equivalently if $T \in \mathcal{B}(\mathcal{H}, \mathcal{H}')$, $T^*T = \mathbb{I}_{\mathcal{H}}$ and $TT^* = \mathbb{I}_{\mathcal{H}'}$.*

(d) *$T \in \mathcal{L}(\mathcal{H}, \mathcal{H})$ is* ***positive*** *if $(v|Tv) \geq 0$ for all $v \in \mathcal{H}$.*[3]

Now, we consider the set of all ~~dense~~ operators. In particular, we want to study the existence of an adjoint for these operators. ~~In this case, the scenario is more complicated. The problem is that the choice~~ of T^*w ~~as in the~~ equation (1.8) ~~could not be unique, and an adjoint operator could not be defined at all~~. In fact, if we take a vector T^*w such that equation (1.8) holds for any $v \in D(T)$, ~~and sum~~ $\cancel{v_0} \in \cancel{D(T)^{\perp}}$, ~~the equation still holds true and~~ $\cancel{T^*}$ ~~could not be a function~~. In order to avoid this problem ~~defining~~ $\cancel{T^*}$, we need to impose our operators to be at least dense so that $D(T)^{\perp} = \emptyset$). In this case:

1.1.13 Definition. *Let $\mathcal{H}$ ~~a~~ Hilbert space, ~~and~~ $T : D(T) \to \mathcal{H}$ a dense operator. Then we call the adjoint operator T^* the operator defined in*

$$D(T^*) = \{v \in \mathcal{H} \mid \exists z_{T,v} \in \mathcal{H} \text{ such that } (v|Tw) = (z_{T,v}|w)\ \forall w \in D(T)\}, \tag{1.10}$$

and which maps $v \mapsto T^*v := z_{T,v}$. Furthermore, T is

(a) ***Hermitian*** *if $\forall v, w \in D(T)$ we have $(v|Tw) = (Tv|w)$,*

(b) ***symmetric*** *if it is Hermitian and $D(T)$ is dense,*

(c) ***self-adjoint*** *if it is symmetric and $T = T^*$,*

(d) ***essentially self-adjoint*** *if $D(T)$ and $D(T^*)$ are dense and $T^* = T^{**}$,*

(e) ***normal*** *if $T^*T = TT^*$ in their standard domain.*

1.1.14 Example. Let us consider the momentum operator $P := -i\partial_x$ as Example 1.1.9. As we said before, P is dense since we could define it over the dense subspace of smooth functions with compact support $C_0^\infty(\mathbb{R})$. Using integration by parts it holds that $\forall f, g \in C_0^\infty(\mathbb{R})$ $(f| - i\partial_x g) = (-i\partial_x f|g)$. Then P is Hermitian as well.

The next concept we have to describe is that of *spectrum* of a linear operator. It is assumed in quantum mechanics that the possible results of a measurement are given by the "eigenvalues" of suitable linear operators. We define the spectrum has the complement of another set of complex numbers called *resolvent set*.

[3]Generally, a positive operator is indicated with "$T \geq 0$"

1.1.15 Definition (**Resolvent and Spectrum**). *Let be T an operator in a normed space X.*

(a) *The resolvent set of T the set $\rho(T)$ containing the values $\lambda \in \mathbb{C}$ such that:*

  (i) $\overline{Ran(T - \lambda\mathbb{I})} = X$,

  (ii) $(T - \lambda\mathbb{I}) : D(T) \to X$ *is injective,*

  (iii) $(T - \lambda\mathbb{I})^{-1} : Ran(T - \lambda\mathbb{I}) \to X$ *is bounded.*

(b) *The spectrum of T is the set $\sigma(T) := \mathbb{C} \setminus \rho(T)$.*
It is the union of the following three sets:

  (i) *the point spectrum of T, $\sigma_p(T)$, containing all $\lambda \in \mathbb{C}$ such that $T - \lambda\mathbb{I}$ is not injective,*

  (ii) *the continuous spectrum, $\sigma_c(T)$, containing all $\lambda \in \mathbb{C}$ such that $T - \lambda\mathbb{I}$ is injective and $\overline{Ran(T - \lambda\mathbb{I})} = X$, but $(T - \lambda\mathbb{I})^{-1}$ is not bounded,*

  (iii) *the residual spectrum, $\sigma_r(T)$, containing all $\lambda \in \mathbb{C}$ such that $T - \lambda\mathbb{I}$, but $\overline{T - \lambda\mathbb{I}} \neq X$.*

1.1.16 Observation. Note that from this definition the spectrum has a more complicate structure than the simple set of all complex numbers λ such that exist a solution v for the equation $Tv = \lambda v$ (the only point spectrum $\sigma_p(T)$).

In our dissertation, the following relation between self-adjoint operators and their spectrum will be useful.

1.1.17 Proposition. *Consider a Hilbert space $\mathcal{H}$ and $T \in \mathcal{B}(\mathcal{H})$. Then, $\sigma(T) \subseteq [-\|T\|, \|T\|]$ holds. Furthermore, if $T = T^*$ we have*

(a) $\sigma(T) \subset [m, M]$, *where* $m = \inf_{\|v\|=1}(v|Tv)$ *and* $M = \sup_{\|v\|=1}(v|Tv)$,

(b) $m, M \in \sigma(T)$,

(c) $\|T\| = \max\{-m, M\}$.

Now, We need to introduce another tool: *projectors*. We will see that evaluating the probability of an outcome from given measure is tantamount to projecting of a state $v \in \mathcal{H}$ on a closed subspace of a $\mathcal{H}$

1.1.18 Definition (**Projector operator**). *Let $\mathcal{H}$ be a Hilbert space and let $P \in \mathcal{B}(\mathcal{H})$ be a bounded operator. P is called an orthogonal projector if $P^2 = P$ and $P = P^*$.*

1.1.19 Observation. An important result linked with projectors operators is the *spectral theorem*. It states that, given a self-adjoint operators, it could be decomposed into an "integral"[4] of projectors, each one associated with an element of the spectrum.

[4] For a more detailed discussion, see [1, Chap. 8]

In quantum mechanics, dynamics is given by Schrödinger equation. General solutions of this equation could be found using the following definition.

1.1.20 Definition. *Let $A \in \mathcal{B}(\mathcal{H})$ where $\mathcal{H}$ is an Hilbert space. Then we define the operator* $\exp(A)$ *as*

$$\exp(A) := \sum_{n=0}^{\infty} \frac{A^n}{n!} \tag{1.11}$$

1.1.21 Observation. The sum reported in Eq. (1.11) must be read as follows: The sequence of partial sums $S_m := \sum_{n=0}^{m} A^n/n!$ converges to an operator in $\mathcal{B}(\mathcal{H})$, i.e. there exists an operator $\exp(A) \in \mathcal{B}(\mathcal{H})$ such that $\lim_{m\to\infty} \|S_m - \exp(A)\| = 0$.

1.1.22 Theorem (Stone's Theorem). *Let H be a Hilbert space. If $T \in \mathcal{B}(\mathcal{H})$ is self-adjoint, then the operators $U_t := \exp(itT)$ (with $t \in \mathbb{R}$):*

(a) form a strongly continuous one-parameter unitary group, i.e. for all $t_0 \in \mathbb{R}$, $\lim_{t\to t_0} U_t = U_{t_0}$ and U_{t_0} is unitary.

(b) if $\psi \in \mathcal{H}$, the limit

$$\partial_t|_{t=0} U_t\psi := \lim_{t\to 0} \frac{U_t\psi - \psi}{t} \tag{1.12}$$

exists;

(c) if $\psi \in \mathcal{H}$:

$$\partial_t|_{t=0}\psi = iT\psi. \tag{1.13}$$

A proof of this theorem is found in [1, Th. 9.33]

1.2 Fourier Transform

The second part of this section will be devoted to the concept of *Fourier transform*. First of all, we need to introduce the class of rapidly-decreasing test function (or Schwartz function) and tempered distributions. Then we will give a definition of Fourier Transform for these spaces and in the end extend this definition to the class of square-summable functions $L^2(\mathbb{R})$.

1.2.1 Definition (Schwartz test function). *Let $f : \mathbb{R} \to \mathbb{C}$ a smooth function. Then, f its called a Schwartz test function (or rapidly decreasing functions) if for all $\alpha, \beta \in \mathbb{N}$ we have $\|f\|_{\alpha,\beta} := \sup_{x\in\mathbb{R}} |x^\alpha \partial_x^\beta f(x)| < +\infty$. This class of functions is indicated with the symbol $\mathcal{S}(\mathbb{R})$. Furthermore, a sequence $\{f_n\} \in \mathcal{S}(\mathbb{R})$ converges in $\mathcal{S}(\mathbb{R})$ if there exists a function $f \in \mathcal{S}(\mathbb{R})$ such that for all $\alpha, \beta \in \mathbb{N}$ we have $\lim_{n\to\infty} \|f_n - f\|_{\alpha,\beta} = 0$. In this case we write $f_n \to f$ ("converges to").*

1.2.2 Observation. The reason we introduce the class of function $\mathcal{S}(\mathbb{R})$ is the following: We want to see the space $L^2(\mathbb{R})$ (which represents the physical wave functions) as linear functional over $\mathcal{S}(\mathbb{R})$.

1.2.3 Definition (Tempered distributions). *Let be $u : \mathcal{S}(\mathbb{R}) \to \mathbb{C}$ be a functional. We call u a temperate distribution if it is continuous with respect to the topology $\mathcal{S}(\mathbb{R})$, in the sense that, for every sequence $\{f_n\} \in \mathcal{S}(\mathbb{R})$ which converges to $f \in \mathcal{S}(\mathbb{R})$, $\lim_{n\to\infty} u(f_n) = u(f)$. We indicate the set of these functionals as $\mathcal{S}'(\mathbb{R})$.*

We need to define the elementary operations for distributions: *derivatives* and *multiplications* with smooth functions.

1.2.4 Definition. *Let $u \in \mathcal{S}'(\mathbb{R})$ and $\alpha \in \mathbb{N}$. We define the α-th derivative[5] of u a distribution $\partial_x^\alpha u \in \mathcal{S}'(\mathbb{R})$ such that*

$$\partial_x^\alpha u(f) = (-1)^\alpha u(\partial_x^\alpha f) \ \forall \alpha \in \mathbb{N}, \ \forall f \in \mathcal{S}(\mathbb{R}). \tag{1.14}$$

We also define the multiplication of a temperate distribution $u \in \mathcal{S}'(\mathbb{R})$ with a smooth function $\varphi \in C^\infty(\mathbb{R})$, the temperate distribution φu defined as

$$\varphi u(f) := u(\varphi f) \ \forall f \in \mathcal{S}(\mathbb{R}). \tag{1.15}$$

Now we have the following proposition

1.2.5 Proposition. *There exists a continuous embedding $L^2(\mathbb{R}) \hookrightarrow \mathcal{S}'(\mathbb{R})$; for all $g \in L^2(\mathbb{R})$ the functional defined in $\mathcal{S}(\mathbb{R})$ as*

$$(g|f) = \int_{-\infty}^{+\infty} \overline{g(x)} f(x)\,\mathrm{d}x, \ \forall \ f \in \mathcal{S}(\mathbb{R}) \tag{1.16}$$

is a tempered distribution.

1.2.6 Observation. The last proposition entails that every square-integrable function generates a continuous functional in this space of rapidly-decreasing test-functions.

1.2.7 Definition (Fourier transform). *Let $f \in \mathcal{S}(\mathbb{R})$. We call the Fourier transform of f:*

$$\widehat{f}(p) \equiv \mathcal{F}[f](p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ipx} f(x)\,\mathrm{d}x. \tag{1.17}$$

On the contrary, if $u \in \mathcal{S}'(\mathbb{R})$, its Fourier transform is the functional $\widehat{u}$:

$$\widehat{u}(f) \equiv \mathcal{F}[u](f) = u(\widehat{f}) \ \forall f \in \mathcal{S}(\mathbb{R}). \tag{1.18}$$

[5] Here α is the order of derivation

1.2.8 Observation. Observe (see [2, Chap. 8]) that for each $f \in \mathcal{S}(\mathbb{R})$ and $u \in \mathcal{S}'(\mathbb{R})$, their Fourier transform also lies respectively in $\mathcal{S}(\mathbb{R})$ and in $\mathcal{S}'(\mathbb{R})$. In addition, there exists an inverse transformation $\mathcal{F}^{-1}$ defined as

$$\mathcal{F}^{-1}[g](x) \equiv \check{g}(x) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ipx} g(p) \, \mathrm{d}p \text{ with } g \in \mathcal{S}(\mathbb{R}), \tag{1.19}$$

$$\mathcal{F}^{-1}[u](f) \equiv \check{u}(f) := u(\check{f}) \text{ with } u \in \mathcal{S}'(\mathbb{R}), \ \forall f \in \mathcal{S}(\mathbb{R}). \tag{1.20}$$

Once we defined $\mathcal{F}$, we state a few important properties;

1.2.9 Theorem. *Let $f \in \mathcal{S}(\mathbb{R})$. Then, we have:*

(a) $\widehat{x^\alpha f}(p) = (-i)^\alpha \partial_p^\alpha \widehat{f}(p) \ \forall \alpha \in \mathbb{N}.$

(b) $\widehat{\partial_x^\alpha f}(p) = (-i)^\alpha p^\alpha \widehat{f}(p) \ \forall \alpha \in \mathbb{N}.$

Now let $u \in \mathcal{S}'(\mathbb{R})$. Then, we have

(c) $\widehat{x^\alpha u} = (-i)^\alpha \partial_p^\alpha \widehat{u} \ \forall \alpha \in \mathbb{N}.$

(d) $\widehat{\partial_x^\alpha u} = (-i)^\alpha p^\alpha \widehat{u} \ \forall \alpha \in \mathbb{N}.$

Proof. For point (a), we only need to re-write the function inside the integral (1.17) $e^{ipx} x^\alpha f(x)$ as $(-i)^\alpha \partial_p^\alpha e^{-ipx} f(x)$ and take the derivative outside the integral. In order to prove point (b), we must use integration by parts and transfer the derivation on f into a derivation on e^{-ipx}. So we can obtain our hypotesis. Point (c) and (d) can be proved by considering the distributions $\widehat{x^\alpha u}$ and $\widehat{\partial_x^\alpha u}$ acting on some test function $f \in \mathcal{S}(\mathbb{R})$, and then using the definitions 1.2.4, 1.2.7 and points (a), (b) to verify our thesis. ∎

1.2.10 Theorem (Plancherel's Theorem). *Let $u \in \mathcal{S}'(\mathbb{R})$. Then $u \in L^2(\mathbb{R})$ if and only if $\widehat{u} \in L^2(\mathbb{R})$. Furthermore, for all $u \in L^2(\mathbb{R})$*

$$\|u\|_{L^2} = \|\widehat{u}\|_{L^2}. \tag{1.21}$$

Then the Fourier transform could be thought as a linear isometric operator in $L^2(\mathbb{R})$.

The proof of this Theorem could be found in [3, Th. 6.1].

1.2.11 Definition (Convolution product). *Let be $f, g \in L^2(\mathbb{R})$. We define the convolution product of f and g the function defined as*

$$f \star g(x) := \int_{-\infty}^{+\infty} f(x-y) g(y) \, \mathrm{d}y \tag{1.22}$$

Once we defined the convolution product, we need to enunciate a theorem that will be useful during the investigation of our thesis.

1.2.12 Theorem (Convolution theorem). *For all $v, u \in L^2(\mathbb{R})$, the following identities holds:*

(i) $\widehat{u \star v} = \widehat{u}\widehat{v}$,

(ii) $\widehat{uv} = (2\pi)^{-\frac{1}{2}}\widehat{u} \star \widehat{v}$

Now we can pass to the final section this first chapter and discuss about the basic concepts of quantum mechanics.

1.3 Quantum Mechanics

1.3.1 Axioms

In the last part of this chapter we are going to investigate the foundations of quantum mechanics. The crucial points about the behavior of quantum systems could be outlined as follows (a more in-depth investigation on the axioms of quantum mechanics is present in [1, Chap. 7]):

(A1) The result of a measurement on a quantum system with fixed state has only probabilistic outcome. It is not possible to know the exact result of a measure (i.e. the position of a particle), but only the probability of each possible result. However, if a physical quantity has been measured, a second measure done immediately after the first one, will give the same result.

(A2) There exist *non-compatible* physical quantities, in the following sense. Consider A, B such quantities and a physical system in a given state. If we first measure A and read the outcome a, and immediately after we make a measurement of B obtaining b, Then a subsequent measuring of A - as close as we want to the measurement of B to avoid ascribing the result to the evolution of the state - will give a value $a_1 \neq a$ in general. Furthermore, it's been seen that incompatible quantities are never functions one of the other and there not exist experimental apparatus able to measure at the same time the two quantities.
There also exist *compatible* quantities in the following sense. Suppose that A' and B' are physical quantities of this type, then we make two successive and arbitrarily close measures of A' and B', obtaining the values a and b respectively. If we make a third measure arbitrarily close to the other two of the quantity A', we will obtain again the value a. And the same happens if we exchange A' with B'. It's has been seen that each quantity A is self-compatible and that if a quantity B is function of another quantity C, then they are compatible.

In Quantum Mechanics measurable quantities whose behavior is ruled by **(A1)** and **(A2)** are called *observables*. In classical mechanics, the counterpart is described as "smooth" functions on the phase space. Instead in quantum mechanics, observables are thought as Hermitian operators defined on a suitable Hilbert space and the physical state of the underlying quantum system is thought as a vector of such space. Hence, we have the following statements:

(A3) Observables correspond to Hermitian operators $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ defined in some Hilbert space $\mathcal{H}$ and all possible results of a measurement are given by the elements of the spectrum $\sigma(A)$.

(A4) The physical state of a quantum system is associated with a vector ψ on this Hilbert space $\mathcal{H}$. This vector gives us all information required to define the distribution probability of all possible outcomes. In fact, the probability of measuring a certain value or set of values $P_\Delta^{(A)}$ (probability that a measure of A gives a number inside the set $\Delta \subseteq \mathbb{R}$) is:

$$P_\Delta^{(A)} := (\psi|P\psi), \tag{1.23}$$

where P is a projector operator on the eigenspace associated with the elements of $\sigma(A)$ lying in Δ. Furthermore, the expectation value $\langle A\rangle$ of A is

$$\langle A\rangle = (\psi|A\psi). \tag{1.24}$$

In addition, a consequence of what said before is that the projector associated to $\mathbb{R}$ is the identity $\mathbb{I}$

$$P_\mathbb{R}^{(A)} = (\psi|\psi) = 1, \tag{1.25}$$

which implies $\|\psi\| = 1$.

1.3.1 Remark. From the last equation we can understand why an observable A has to be an Hermitian operator. Since the result of our measurements are real numbers, we want $\langle A\rangle \in \mathbb{R}$ and $\sigma(A) \subseteq \mathbb{R}$, but these conditions are implied by the fact that A is Hermitian.

1.3.2 Observation. The existence of projectors as in (1.23) is guaranteed by the *spectral theorem*. More precisely, it states that for any self-adjoint operator A there exists a one-parameter family of projectors that associates an element, or a subset, of $\sigma(A)$ the orthogonal projector into the corresponding eigenspace.

1.3.3 Example. Let us consider the "position" operator defined in Ex. 1.1.9. It is an operator $X : D(X) \to L^2(\mathbb{R})$ with $D(X) = C_0^\infty(\mathbb{R})$, which maps $f \mapsto xf$. It is called the "position" operator because it is really the Hermitian and symmetric operator associated with the measure of the position of a particle. A particle instead is described by a $\psi \in L^2(\mathbb{R})$ (also called "wave function") such that

$$\|\psi\|_{L^2}^2 = \int_{-\infty}^{+\infty} |\psi(x)|^2 \,\mathrm{d}x = 1. \tag{1.26}$$

Here $|\psi(x)|^2$, following statement **(A4)**, has the value a of density probability function for the position of the particle. Moreover, the projector operator associated with a certain interval $(a, b) \subset \mathbb{R}$ is the characteristic function $\chi_{(a,b)}$[6] and the probability of finding the particle within the interval (a, b) is:

$$P_{\Delta}^{(X)} = (\psi|\chi_{(a,b)}\psi) = \int_{-\infty}^{+\infty} \chi_{(a,b)}(x)|\psi(x)|^2 \,\mathrm{d}x = \int_a^b |\psi(x)|^2 \,\mathrm{d}x. \tag{1.27}$$

The expectation value of X is given by:

$$\langle X \rangle = (\psi|X\psi) = \int_{-\infty}^{+\infty} x|\psi(x)|^2 \,\mathrm{d}x. \tag{1.28}$$

1.3.4 Example. Another example is the "momentum" operator $P := -i\partial_x$ defined in $D(P) = C_0^\infty(\mathbb{R})$. Using integration by parts, one can prove that P is Hermitian and symmetric. As well as X is the operator associated to a position measurement, so P is the operator associated to the physical quantity of momentum and it is defined in the same Hilbert space of X. Its expectation value is

$$\langle P \rangle = (\psi|P\psi) = -i \int_{-\infty}^{\infty} \psi^*(x)\partial_x\psi(x) \,\mathrm{d}x \tag{1.29}$$

Note that if we take the Fourier transform of a wave function $\psi \in L^2(\mathbb{R})$ we have (using Th. 1.2.9)

$$P\psi = P\mathcal{F}^{-1}\mathcal{F}\psi = \frac{-i}{\sqrt{2\pi}}\partial_x \int_{-\infty}^{+\infty} e^{ipx}\widehat{\psi}(p) \,\mathrm{d}p = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ipx} p\widehat{\psi}(p) \,\mathrm{d}p, \tag{1.30}$$

while

$$\langle P \rangle = (\mathcal{F}^{-1}\mathcal{F}\psi|P\mathcal{F}^{-1}\mathcal{F}\psi) = (\mathcal{F}^{-1}\mathcal{F}\psi|\mathcal{F}^{-1}\mathcal{F}\widehat{P}\psi) = \int_{-\infty}^{\infty} p|\widehat{\psi}(p)|^2 \,\mathrm{d}p, \tag{1.31}$$

where we defined $\widehat{P} : \phi(p) \mapsto p\phi(p)$. This entails that P could be transformed from a derivative operator in one space (which could be called the "position" space), to a multiplicative operator $\widehat{P}$ in the transformed space (called the "momentum" space). The same thing could be said in the opposite way for the operator X.

1.3.5 Remark. Considering particles of mass $m > 0$, it will be convenient to work with dimensionless variables x, p, etc., and dimensionless functions by using a length scale ℓ as the unit of length, $\hbar/\ell$ as the unit of momentum, $m\ell^2/\hbar$ as the unit of time, and $\hbar^2/m\ell^2$ as the unit of energy, effectively setting $m = \hbar = 1$.

[6] $\chi_{(a,b)}$ is the function which maps to zero outside (a, b) and one inside

1.3.2 Dynamics

We now focus on the time evolution of a physical system. We are interested in the equation which determines how the vector ψ, which describes the underlying system, evolves in the Hilbert space when the system is interacting. This role, in non-relativistic quantum mechanics, is played by *Schrödinger equation*. Hence we have

(A5) The time evolution of a physical state, described by a vector ψ in a Hilbert space $\mathcal{H}$ is given by the *Schrödinger equation*

$$i\partial_t\psi = H\psi \tag{1.32}$$

where H is the Hamiltonian operator, it is Hermitian and it represents the energy of a physical system. We can write its expectation value as

$$\langle H\rangle = (\psi|H\psi). \tag{1.33}$$

In the case of particles which travel in the physical space under the action of a potential $V(x)$, the Hilbert space $L^2(\mathbb{R})$[7], the Hamiltonian H is

$$H := \frac{1}{2}P^2 + V(X) \tag{1.34}$$

where $P^2/2$ is the "kinetic energy" operator while $V(X)$ is the operator $\psi \mapsto V(X)\psi := V(x)\psi(x)$. Here H could be interpreted as the energy of a unit mass particle which travels in a potential well ruled by V.

Now we want to find a general solution for Schrödinger equation. In particular, given a fixed initial state $\psi(0)$ for our physical system, we want to determine the final state at a certain time $\psi(t)$. In order to find these solutions, we must resume Def. 1.1.20 for exponential operators and Stone's Theorem 1.1.22.
Given an Hamiltonian H, let us consider the operator

$$U(t) := \exp(-iHt) = \sum_{n=0}^{\infty}\frac{(iHt)^n}{n!} \tag{1.35}$$

and suppose that this sum is well-defined. $U(T)$ is called *unitary evolution operator* and it indicates how a fixed initial state evolve with time. In fact, if we take $\psi_0 \in \mathcal{H}$ with $\|\psi_0\| = 1$ as initial state, Then, according to Stone's theorem, $\psi_t := U(t)\psi_0$ is the solution of our Schrödinger equation since

$$i\partial_t\psi_t = i\partial_t\exp(-iHt)\psi_0 = i(-iH)\exp(-iHt)\psi_0 = H\psi_t. \tag{1.36}$$

It could be seen that $U(t)$ is Hermitian and that $U(t)^*U(t) = \mathbb{I}$ (from here the term *unitary*). Hence

$$\|\psi_t\|^2 = (U(t)\psi_0|U(t)\psi_0) = (\psi_0|U(t)^*U(t)\psi_0) = \|\psi_0\|^2 = 1. \tag{1.37}$$

[7]For particles moving in three dimensions we consider $L^2(\mathbb{R}^3)$

1.3.6 Definition. *Let $\psi \in L^2(\mathbb{R})$. Then the density probability current is*

$$j_\psi(x,t) := \frac{1}{2i}[\partial_x\psi(x,t)\psi^*(x,t) - \psi(x,t)\partial_x\psi^*(x,t)], \tag{1.38}$$

This quantity gives us information how probability flows in space and it is bounded with the density probability function $\rho(x,t) := |\psi(x,t)|^2$ by the *continuity equation*

$$\partial_t\rho(x,t) + \partial_x j_\psi(x,t) = 0. \tag{1.39}$$

Now, we turn back to our physical particles described by square-integrable functions and consider the Hamiltonian H_0 given by only the kinetic term of equation (1.34) $H_0 = P^2/2$. This Hamiltonian represents the evolution of free particles which are not subjected by any external potential. We note that in this case, solutions given by $U(t)\psi_0 = \exp(-iH_0t)\psi_0$ have a simple form. Since the derivative operator P could be transformed to a multiplicative operator in the Fourier-transformed space, then the exponential operator $\exp(-iP^2t/2)$ could be seen as a multiplicative phase in the "momentum" space.

$$\exp(-iP^2t/2)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ipx}\widehat{\psi_0}(p)\,\mathrm{d}p = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ip(x-pt/2)}\widehat{\psi_0}(p)\,\mathrm{d}p \tag{1.40}$$

In presence of a generic potential $V(x)$, complications arise. In this case it is helpful to introduce the *interaction picture*[8]. We consider an Hamiltonian

$$H = H_0 + V(X) \tag{1.41}$$

where $H_0 = P^2/2$. Given a solution of the Schrödinger equation $\psi(t)$, with initial condition $\psi(0) = \psi_0$, we define

$$\psi_I(t) := e^{iH_0t}\psi(t)\,, \tag{1.42}$$

where $\psi_I(t)$ stands for a state that represents the same physical situation in *interacting picture*. At $t = 0$, $\psi_I(0) = \psi(0) = \psi_0$. On the contrary, we define observables in the interacting picture as

$$A_I = e^{iH_0t}Ae^{-iH_0t}\,, \tag{1.43}$$

where A is the operator associated with the observable. In particular,

$$V_I(X) = e^{iH_0t}V(X)e^{-iH_0t}\,, \tag{1.44}$$

where $V(X)$ is the potential in (1.41). To derive the fundamental solution that characterized the evolution of a state in interacting picture, consider the derivative of (1.42)

$$\begin{aligned} i\partial_t\psi_I(t) &= i\partial(e^{iH_0t}\psi(t)) \\ &= -H_0e^{iH_0t}\psi(t) + e^{iH_0t}(H_0 + V(X))\psi(t) \\ &= e^{iH_0t}V(X)e^{-iH_0t}e^{iH_0t}\psi(t)\,. \end{aligned} \tag{1.45}$$

[8] see [4, Chap. 5, Sect. 5]

Thus, we have

$$i\partial_t \psi_I(t) = V_I(X)\psi_I(t)\,. \tag{1.46}$$

1.3.7 Observation. (1.46) is a Schrödinger-like equation with total Hamiltonian H replaced by $V_I(X)$. Stated differently, $\psi_I(t)$ would be a fixed vector in his Hilbert space if $V_I = 0$. We can also show for an observable A (which does not depends explicitly with time) that

$$\partial_t A_I = -i[A_I, H_0]\,. \tag{1.47}$$

At this point, we wonder what relation lies between the solutions of the interacting and the free scenario[9]. To do this, we consider an Hamiltonian $H = H_0 + V$, as in (1.41), and one particle, initially free, which scatters against the potential V. Stated differently, we can say that the system is prepared at $t \to -\infty$ in an approximately free state, and after interaction, as $t \to \infty$, it manifests itself in a state that can still be seen as free.
The fact that for certain state vectors, indicated at $t = 0$ by ψ_0, the evolution in time is approximated by the non-interacting evolution in the far future and past, is expressed by

$$\lim_{t\to\pm\infty} \|e^{-itH}\psi_0 - e^{-itH_0}\phi_\pm\| = 0\,, \tag{1.48}$$

for some state $\phi_\pm$. Equivalently

$$\lim_{t\to\pm\infty} \|\psi_0 - e^{itH}e^{-itH_0}\phi_\pm\| = 0\,. \tag{1.49}$$

In scattering theory, it is convenient to describe interactions using vectors like $\phi_\pm$, that evolve by the Hamiltonian of the non-interacting theory, rather than ψ_0, which evolves with the interacting Hamiltonian H. This motivets us to introduce the *Møller operators* $\Omega_V^\pm$.

1.3.8 Definition. *Let $H_0 = P^2/2$ the free Hamiltonian and $H = P^2/2 + V(X)$ an interacting Hamiltonian for some potential V. We define* ***Møller operators*** $\Omega_V^\pm$ *as:*

$$\Omega_V^\pm := \lim_{t\to\pm\infty} e^{iHt}e^{-iH_0t} \tag{1.50}$$

1.3.9 Observation. If the operators $\Omega_V^\pm : \mathcal{H} \to \mathcal{H}$ exist they must be isometries, since they are limits of unitary operators. More precisely, they are isometries with initial space $\mathcal{H}$ and final space

$$\mathcal{H}_\pm := \mathrm{Ran}(\Omega_V^\pm)\,. \tag{1.51}$$

It can be proved that $\mathcal{H}_\pm$ are closed subspace of $\mathcal{H}$.

[9]For a more detailed discussion, see [1, Chap. 13, Sect. 1.5]

By construction, if $\phi \in \mathcal{H}$, it holds

$$\|e^{-itH}\psi_\pm - e^{-itH_0}\phi\| \to 0 \text{ as } t \to \pm\infty \tag{1.52}$$

for some $\psi_\pm \in \mathcal{H}_\pm$, such that $\psi_\pm = \Omega_V^\pm \phi$. Hence $\mathcal{H}$ indicates the class of states whose long time future evolution, or long-time past evolution, can be approximated by the free evolution of the states obtained swapping the $\Omega_V^\pm$. (1.52) tells us that the state of the interacting system $\psi_\pm$ has the asymptotic behavior (as $t \to \pm\infty$, respectively) of the state ϕ in the non-interacting system.
Following, we enunciate some fundamental properties for the Møller operators.

1.3.10 Theorem. *Let H_0 and H be the Hamiltonian in Definition 1.3.8, and let $\Omega_V^\pm : \mathcal{H} \to \mathcal{H}_\pm$ exist. Then*

(a) $e^{-itH}\Omega_V^\pm = \Omega_V^\pm e^{-itH_0}$.

(b) $\Omega_V^{\pm\,*} = \lim_{t\to\pm\infty} e^{iH_0 t} e^{-iHt}$ *if the limit in the right hand side exists*[10].

1.3.11 Remark. In the following discussion, we will restrict us to consider the only Ω_V^-. Hence we set $\Omega_V^- \equiv \Omega_V$ in order to simplify the notation.

[10] see [15, Th. 3.5]

Chapter 2

Quantum Backflow - Basic Concepts

In this chapter we start our discussion on the backflow effect. First of all, we will give an historical introduction on the first observations and subsequently we dwell into a deeper analysis. Then, we will give a rigorous definition of backflow reporting a few illustrative and relevant examples. In the central part of this chapter we will focus on outlining the basic properties of backflow in free field theories. For this purpose, we shall retrace the first work of Braken and Melloy [6], outlining its most important results and discussing in detail and rigorously their results.
As we remarked in Section 1.3, considering particles of mass $m > 0$, it will be convenient to work with dimensionless variables for position x, momentum p, etc., and dimensionless functions (such as the wave function ψ and the current j_ψ) by using a length scale ℓ as the unit of length, $\hbar/\ell$ as the unit of momentum, $m\ell^2/\hbar$ as the unit of time, and $\hbar^2/m\ell^2$ as the unit of energy, effectively setting $m = \hbar = 1$.

2.1 Historical Introduction

Let us start by contextualizing the problem from which quantum backflow arises. Consider a particle bounded to travel freely on a straight line. According to Section 1.3, all particles are described by a wave function $\psi(x,t)$ whose square of absolute value $|\psi(x,t)|^2$ gives the probability density of finding the particle at some point of space x and at some time t. At the same time, if we take the Fourier transform, $\widehat{\psi}(p,t)$, its square of absolute value $|\widehat{\psi}(p,t)|^2$ gives the density probability of finding the particle with a given momentum p.
Suppose to shoot such a quantum particle with a given positive velocity along the straight line. Hence $\widehat{\psi}(p) \neq 0$ only if $p > 0$. Now consider the probability $P(t)$ of finding the particle behind a certain point, say for definiteness the origin $x = 0$, at a given time t:

$$P(t) := \int_{-\infty}^{0} |\psi(x,t)|^2 \, \mathrm{d}x \tag{2.1}$$

Consider the following question:

For each wave function with strictly positive momentum, is the quantity $P(t)$ always decreasing over time?

Classically, the answer is obvious. If you consider a particle with positive velocity, its position certainly increases with time. Instead in Quantum Mechanics, the outcome is more exotic and wave functions with positive velocity, but increasing $P(t)$ exist. This is *quantum backflow*.
First analysis of this phenomenon date back to 1969 in a work written by Allcock [5] on the problem of time arrival as a physical observable in quantum mechanics. After that, backflow has been neglected until 1994, when Bracken and Melloy made an exhaustive investigation outlining the fundamental properties and quantitative bounds in free theory. Subsequently, Eveson, Fewster and Verch [8] described backflow as a fundamental quantum inequality and in 2013 Palmero [9] gave suggestion for an experimental observation using Bose-Einstein condensate. The analysis of the results obtained by Bracken and Melloy will be discussed in this chapter while the next one will discuss mainly the study of backflow in scattering theory (particles subjected to a potential) treated in the recent work of Bostelmann, Cadamuro and Lechner [7].

2.2 Definition of Backflow and Illustrative Examples

The first goal of this section is to give a complete set of definitions in order to clarify the nature of backflow and the mathematics the lies behind it. We start by clarifying our notion of particles with only positive momentum by introducing the concept of *right-movers.*

2.2.1 Definition (Right-mover). *Let $\psi \in L^2(\mathbb{R})$ be a wave-function associated to a physical quantum particle and let $|\psi(x)|^2$ be the density probability.. We call ψ is called a right-mover if* supp $\widehat{\psi} \in [0, +\infty)$.

2.2.2 Observation. It could be seen that the set of all right-movers is a closed subspace of the Hilbert space $L^2(\mathbb{R})$. Hence, we define a projector operator which transforms each wave-function into a right-mover.

2.2.3 Definition. *We call $E_\pm : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ the operator such that:*

$$\mathcal{F}[E_\pm\psi](p) = \vartheta(\pm p)\widehat{\psi}(p) \ \forall\psi \in L^2(\mathbb{R}), \tag{2.2}$$

where ϑ is the Heaviside function defined as:

$$\vartheta(p) = \begin{cases} 0 & p \leq 0 \\ 1 & p > 0 \end{cases} . \tag{2.3}$$

2.2.4 Observation. This operator takes the representation of the wave-function in momentum space and removes all negative (positive in case of E_-) velocities. We can prove that $E_\pm$ is a real projector in the sense of the Definition 1.1.18.

2.2.5 Proposition. *Let E_+ as in Definition 2.2.3. Then, E_+ is bounded, self-adjoint and $E_+^2 = E_+$.*

Proof. Boundedness is a consequence of Plancherel's Theorem. In fact, for all $\psi \in L^2(\mathbb{R})$ with $\|\psi\| = 1$

$$\|E_+\psi\| = \|\mathcal{F}[E_+\psi]\| = \|\vartheta\widehat{\psi}\| \leq \|\widehat{\psi}\| = \|\psi\| = 1 \tag{2.4}$$

Self-adjointness is a by-product of the properties of the Fourier transform

$$(\psi|E_+\phi) = (\widehat{\psi}|\widehat{E_+\phi}) = (\widehat{\psi}|\vartheta\widehat{\phi}) = (\vartheta\widehat{\psi}|\phi) = (E_+\psi|\phi)\ \forall\phi,\psi \in L^2(\mathbb{R}), \tag{2.5}$$

while $E_+^2 = E_+$ holds per construction. ∎

Note that from this definition we can re-define equivalently every right-mover as those wave-functions ψ such that $E_+\psi = \psi$. Henceforth, we will write the set of all right-movers with the symbol $E_+(L^2)$.
Once we have introduced these concepts, we are able to give an exhaustive definition of backflow:

Given a right-mover $\psi = E_+\psi$, backflow occurs whenever the density probability current function $j_\psi = -i/2[\psi^*\partial_x\psi - \psi\partial_x\psi^*]$ assumes negative values.

2.2.6 Observation. The fact that the density current assumes negative values in some point $x \in \mathbb{R}$ is equivalent to the increasing of the probability of finding the particle in $(-\infty, x)$. In fact, if we set $x = 0$

$$\begin{aligned}\dot{P}(t) &= \partial_t \int_{-\infty}^{0} |\psi(x,t)|^2 \,\mathrm{d}x \\ &= \int_{\infty}^{0} (\partial_t\psi(x,t)\psi^*(x,t) + \psi(x,t)\partial_t\psi^*(x,t))\,\mathrm{d}x \\ &= \int_{-\infty}^{0} (-i\psi^*(x,t)H_0\psi(x,t) + i\psi(x,t)H_0\psi^*(x,t))\,\mathrm{d}x \\ &= -j_\psi(0,t)\,,\end{aligned} \tag{2.6}$$

where we used integration by parts and the Schrödinger equation with the Hamiltonian of free particle $H_0 = P^2/2 = -\partial_x^2/2$.

At this point, we are interested in showing clearly that backflow is a truly quantum effect predicted by the non-relativistic mono-dimensional Schrödinger equation. to this avail, we will illustrate some examples in which backflow occurs.

2.2.1 Superposition of Plane Waves

The first instructive example is given by:

$$\begin{aligned} &\psi(x,t) = Ae^{i\vartheta_1(x,t)} + Be^{i\vartheta_2(x,t)}, \\ &\text{where } \vartheta_n(x,t) = \left[p_n\left(x - \frac{p_n t}{2}\right) + \gamma_n\right] \quad n = 1,2. \end{aligned} \tag{2.7}$$

Here we choose A, B, p_1 and p_2 positive constants, while γ_1 and γ_2 are arbitrary real numbers. Eq. (2.7) is the sum of two plane waves, eigenfunctions of the free-particle Hamiltonian, with positive momentum p_n and energy $p_n^2/2$ for $n = 1, 2$. This does not represent a real state because it is not normalizable. Nevertheless it could be interesting to study how backflow could emerge from such a simple case. In fact, we can evaluate the density probability current $j_\psi(x,t)$ at a certain point $x \in \mathbb{R}$ and at the instant $t \in \mathbb{R}$. Remembering Definition 1.3.6 for $j_\psi(x,t)$ we obtain:

$$j_\psi(x,t) = A^2 p_1 + B^2 p_2 + AB(p_1 + p_2)\cos(\vartheta_1(x,t) - \vartheta_2(x,t)). \tag{2.8}$$

We can check that $\vartheta_1(x,t) - \vartheta_2(x,t)$ is linearly dependent with the time t. Hence the density current could vary from an upper value of $(p_1A + p_2B)(A + B)$ to a lower value of $(p_1A - p_2B)(A - B)$. If, for example $A > B$ and $p_1A < p_2B$, this lower value is negative and so backflow occurs.

Although this example has no physical interpretation, because of the non-normalizability of plane waves, we can note that backflow is essentially an interference effect between some wave-packets with high positive momentum and others with low positive momentum. This aspect is not trivial and we will we re-use it for proving an important theorem regarding the intensity of backflow through a single point at a some instant of time. In particular, we will construct a normalized wave-packet in momentum space as a sum of a function $\tilde{\chi}(p) \in L^2(\mathbb{R}_+)$ and its translation $\tilde{\chi}(p - n)$, with $n \in \mathbb{N}$. This coincides with taking the interference of two wave-packets with different positive momenta.

2.2.2 Superposition of Gaussian Wave-packets

Another example can be made by replacing the two plane waves with Gaussian functions tightly picked in momentum. This represents a more physically realistic state. We consider the sum of two initial Gaussian wave-packets with equal spatial width σ, evolved for a time t. The corresponding normalized wave function is

$$\psi(x,t) = \sum_{n=1,2} C_n \frac{1}{\sqrt{4\sigma^2 + 2it}} \exp\left(ip_n(x - p_n t) - \frac{(x - p_n t)^2}{4\sigma^2 + 2it}\right),$$

$$C_n \in \mathbb{R},\ \ p_1, p_2 > 0. \tag{2.9}$$

This function was proposed by Yearsley in [10]. As in the previous example, this wave-function is given by the superposition of two waves with different momentum.

Note that as $\sigma \to 0$, we obtain once more a superposition of plane waves. To prove that for such a function backflow occurs, we set the parameters p_1, p_2, C_1, C_2 and σ to be

$$p_1 = 0.3,\ p_2 = 1.4,\ C_1 = 1.8,\ C_2 = 1,\ \sigma = 10. \tag{2.10}$$

We plot the probability $P(t)$ of the particle being localized at a point $x < 0$ as a function of time, see Figure 2.2. Observe that $P(t)$ is non monotonically decreasing, but in several disjoint time intervals it increases, proving the presence of backflow.

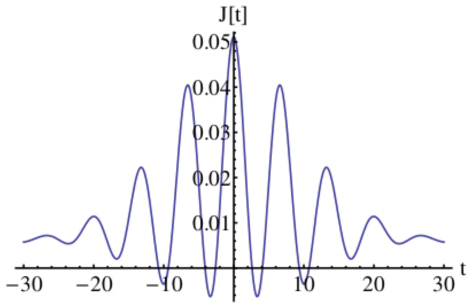

FIGURE 2.1: Plot of the current for a superposition of two gaussians, with the parameters given in Eq. [2.10].

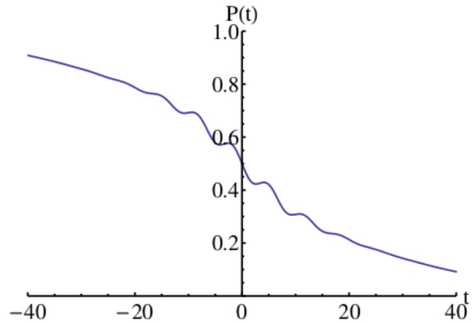

FIGURE 2.2: Plot of the probability for remaining in $x < 0$ for a superposition of two gaussians, with the parameters given in Eq. [2.10].

One might wonder how to quantify the amount of backflow that this state displays. To answer this query, we need to evaluate

$$P(t_1) - P(t_2) = \int_{t_1}^{t_2} j_\psi(0,t)\,\mathrm{d}t, \tag{2.11}$$

where P is the probability of finding the particle within the domain $x < 0$ while $[t_1, t_2]$ is the interval maximizing the amount of backflow for this wave-function. A direct evaluation shows that,

$$F := \inf\{P(t_1) - P(t_2) \mid t_2 > t_1\} \approx -0.0061 \tag{2.12}$$

We will see in the following discussion that this flux is approximately the 16% of the maximum amount of backflow theoretically allowed.

2.2.3 Normalizable Wave

The following example shows that backflow can also occur for normalizable wave-functions. Let us consider $\phi \in L^2(\mathbb{R})$ whose representation in the momentum space (which is nothing more than its Fourier transform $\widehat{\phi}$) is given by the following equation:

$$\widehat{\phi}(p) = \begin{cases} \frac{18}{\sqrt{35K}} p(e^{-p/K} - \frac{1}{6}e^{-p/2K}) & p > 0 \\ 0 & p \leq 0 \end{cases} \tag{2.13}$$

where K is a positive constant. This represents a possible initial state for a physical particle. Now we can write the expression for the function ϕ defined in the position space:

$$\phi(x) = 18\sqrt{\frac{K}{70\pi}} \left[\frac{1}{(1 - iKx)^2} - \frac{2}{3(1 - 2iKx)^2} \right]. \tag{2.14}$$

At this point we can evaluate $\phi(0)$, $\phi'(0)$ and the density probability current $j_\phi(0)$ as:

$$\begin{aligned} &\phi(0) = 6\sqrt{\frac{K}{70\pi}} \qquad\qquad \phi'(0) = -12i\sqrt{\frac{K}{70\pi}} \\ &j_\phi(0) = -\frac{36K^2}{35\pi} < 0, \end{aligned} \tag{2.15}$$

which proves the presence of backflow. Evaluating the time evolution of this wave-function, the current is negative during the interval $[0, t_1]$ where $t_1 \approx 0.021/K^2$. The corresponding flux (from Eq.(2.11)) is

$$F \approx -0.0043 \tag{2.16}$$

2.3 Backflow in Free Theory

In this section we want to study the length and the strength of this effect in the case of free particles. In particular, The question we ask ourselves is:

What is the maximum amount of probability which could flow back through a point x_0 during an interval of time T for a right-moving free-particle?

We will show that this problem is equivalent to finding the smallest eigenvalue of a suitable integral operator, out of which one establish a bound for quantum backflow. In the following discussion we will interpret the flux of probability defined in Eq. (2.11) in a time interval $[0, T]$ through a certain point ,say the origin $x = 0$, as a scalar product of the form $(\widehat{\psi}|\vartheta B_T \vartheta \widehat{\psi})$, where $\widehat{\psi}$ is the Fourier transform of the wave-function (i.e. right-mover), ϑ is the Heaviside function and B_T is the *backflow operator* that will be proved to be bounded and self-adjoint. After that, we will link the upper bound for this operator to the evaluation of the maximum eigenvalue of an integral operator K (defined by Bracken and Melloy in [6]). Furthermore, we will show that this maximum eigenvalue corresponds to the maximum amount of backflow allowed for any right-mover. In this part of our thesis will report the results obtained by Penz *et al.* in [12].

2.3.1 Temporal Boundedness of Backflow

Let us start by considering how the free Schrödinger evolution operator acts in momentum space. We have shown in Section 1.3 that for a wave-function represented in the Fourier-transformed space $\widehat{\psi}$, the evolution operator U_t could be transformed into a phase multiplicative operator:

$$\widehat{\psi}_t(p) = \widehat{U_t\psi} = (\widehat{U}_t\widehat{\psi})(p) = e^{-ip^2t/2}\widehat{\psi}(p)\,, \tag{2.17}$$

where we introduced the operator $\widehat{U}_t := \mathcal{F}U_t\mathcal{F}^{-1}$.

2.3.1 Observation. Notice that, if $\psi \in E_+L^2(\mathbb{R})$, then, by definition of $\widehat{U}_t$, $U_t\psi \in E_+L^2(\mathbb{R})$ for all $t \in \mathbb{R}$. Stated differently, the evolution preserves the subspace $E_+L^2(\mathbb{R})$ of right-mover wave-functions. Furthermore, we observe that $U_t^* = U_{-t}$ and $\widehat{U}_t^* = \widehat{U}_{-t}$.

The representation of such wave-functions in the "position" space are given by the anti-Fourier transform:

$$\psi_t(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ipx}\widehat{\psi}_t(p)\,\mathrm{d}p. \tag{2.18}$$

Let a particle be described in momentum space by a wave-function $\widehat{\psi}(p)$ at time 0. If $\|\widehat{\psi}\| = \|\psi\| = 1$, the probability that a position measurement at time t yields a position $x > 0$ reads

$$L(\psi_t) := \int_0^{+\infty} |\psi_t(x)|^2\,\mathrm{d}x = (\widehat{\psi}|\widehat{U}_t^*\mathcal{F}\vartheta\mathcal{F}^{-1}\widehat{U}_t\widehat{\psi}). \tag{2.19}$$

Now we restrict to consider right-moving wave-functions ψ such that $E_+\psi = \psi$ or equivalently $\vartheta\widehat{\psi} = \widehat{\psi}$ and $\|\psi\| = 1$. Note that for such functions the evolution ψ_t is also a right-mover, $\psi_t = E_+\psi_t$.
As shown in the previous examples, there exist right-moving wave-functions in which backflow occurs and the probability $L(\psi_t)$ does decrease in a time interval. So, it is convenient to define the maximum backflow for a fixed right-mover ψ as

$$\lambda(\psi) = \{L(\psi_s) - L(\psi_t) \mid \psi = E_+\psi,\ \|\psi\| = 1,\ t > s\} \tag{2.20}$$

Since we are interested in the maximum amount of probability backflow, we define the **backflow constant** λ as

$$\lambda := \sup\{\lambda(\psi) \mid \psi = E_+\psi,\ \|\psi\| = 1\}. \tag{2.21}$$

Introducing the orthogonal projector $\tilde{\vartheta}_t := \widehat{U}_t^*\mathcal{F}\vartheta\mathcal{F}^{-1}\widehat{U}_t$ we obtain for any normalized wave-function $\psi \in L^2(\mathbb{R})$

$$L(\psi_s) - L(\psi_t) = (\widehat{\psi}|(\tilde{\vartheta}_s - \tilde{\vartheta}_t)\widehat{\psi}). \tag{2.22}$$

Since

$$\tilde{\vartheta}_s - \tilde{\vartheta}_t = \widehat{U}^*_{\frac{t+s}{2}} (\tilde{\vartheta}_{\frac{s-t}{2}} - \tilde{\vartheta}_{\frac{t-s}{2}}) \widehat{U}_{\frac{t+s}{2}}, \tag{2.23}$$

we can write

$$\lambda = \sup\{(\widehat{\psi}|\widehat{U}^*_\tau(\tilde{\vartheta}_{-T} - \tilde{\vartheta}_T)\widehat{U}_\tau\widehat{\psi}) \mid \psi = E_+\psi,\ \|\psi\| = 1,\ \tau \in \mathbb{R},\ T > 0\}, \tag{2.24}$$

2.3.2 Definition. *Given a fixed time $T > 0$, we call* ***backflow operator*** $B_T : L^2(\mathbb{R}) \to L^2(\mathbb{R})$

$$B_T := \tilde{\vartheta}_{-T} - \tilde{\vartheta}_T. \tag{2.25}$$

B_T enjoys the following properties

2.3.3 Proposition. *The operator $\vartheta B_T \vartheta$ with B_T defined in (2.25) is bounded and self-adjoint.*

Proof. The boundedness of $\vartheta B_T \vartheta$ follows from the boundedness of ϑ and $\widehat{U}_T$ forall $T \in \mathbb{R}$. One can prove self-adjointness by considering the scalar product $(\psi|\vartheta B_T \vartheta \phi)$ for some $\psi, \phi \in L^2(\mathbb{R})$ and see that it is equal to $(\vartheta B_T \vartheta \psi|\phi)$ using self-adjointness of ϑ and the definition of adjoint for $\widehat{U}_T$. ■

2.3.4 Observation. Note that the operator ϑ here needs to cut the negative momenta of a wave-function transforming it into a right-mover.

Focusing on the analysis of the backflow constant λ, since $\widehat{U}_\tau$ preserves the set of right-movers $E_+(L^2)$, see Observation 2.3.1, it holds

$$\lambda = \sup\{(\phi|\vartheta B_T \vartheta \phi) \mid \phi \in L^2(\mathbb{R}),\ \|\phi\| = 1,\ T > 0\}, \tag{2.26}$$

or equivalently

$$\lambda = \sup \bigcup_{T>0} \sigma(\vartheta B_T \vartheta). \tag{2.27}$$

2.3.5 Observation. (2.27) could be simplified by neglecting the set sum over $T > 0$. In fact we see that $\vartheta B_T \vartheta$ is the operator which gives the flux of probability through the origin $x = 0$ for a time interval $[0, T]$. Using scaling arguments, one shows that backflow is independent from the time T, in the sense that, for every right-mover with some amount of backflow during the interval $[0, T]$, there exists another right-mover with the same backflow, but for a time interval $[0, T']$ arbitrarily larger.

2.3.6 Proposition. *For any fixed time $T > 0$, $\lambda = \sup \sigma(\vartheta B_T \vartheta)$.*

Proof. Consider the family of unitary operators $V_\mu : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ with $\mu > 0$ defined as $(V_\mu \phi)(p) := \sqrt{\mu}\phi(\mu p)$. For any $\phi \in L^2(\mathbb{R})$

$$(\vartheta V_\mu \phi)(p) = \sqrt{\mu}\vartheta(p)\phi(\mu p) = \sqrt{\mu}\vartheta(\mu p)\phi(\mu p) = (V_\mu \vartheta \phi)(p), \tag{2.28}$$

and

$$\mathcal{F}\vartheta\mathcal{F}^{-1}V_\mu\phi = \mathcal{F}\vartheta V_{1/\mu}\mathcal{F}^{-1}\phi = \mathcal{F}V_{1/\mu}\vartheta\mathcal{F}^{-1}\phi = V_\mu\mathcal{F}\vartheta\mathcal{F}^{-1}\phi. \tag{2.29}$$

Then V_μ commutes with both the operator ϑ and $\mathcal{F}\vartheta\mathcal{F}^{-1}$. Note that $V_\mu^* = V_{1/\mu}$. A direct calculation shows that

$$V_\mu \widehat{U}_t V_\mu^* = \widehat{U}_{\mu^2 t} \tag{2.30}$$

It follows that

$$V_\mu \vartheta B_T \vartheta V_\mu^* = \vartheta B_{\mu^2 T}\vartheta. \tag{2.31}$$

Since the spectrum of an operator is invariant under a unitary transformation we have for any $T_1, T_2 > 0$

$$\sigma(\vartheta B_{T_1}\vartheta) = \sigma(V_{\mu'}\vartheta B_{T_1}\vartheta V_{\mu'}^*) = \sigma(\vartheta B_{T_2}\vartheta) \quad \text{where} \quad \mu' = \sqrt{T_2/T_1}. \tag{2.32}$$

Hence we can write $\lambda = \sup\sigma(\vartheta B_{T_1}\vartheta)$ for any fixed $T > 0$. ∎

Summing up all results we obtained for the backflow operator B_T and for the backflow constant λ, it holds.

2.3.7 Theorem (Temporal Boundedness of Backflow). *Let $\lambda = \sup\sigma(\vartheta B\vartheta)$, where $B = B_{T=1}$ is the backflow operator. For any right-mover $\psi \in L^2(\mathbb{R})$ such that $\psi = E_+\psi$ and for any $T > 0$ it holds*

$$\int_0^T j_\psi(0,t)\,\mathrm{d}t \geq -\lambda > -\infty. \tag{2.33}$$

Proof. Since λ is the maximum amount of backflow, we must to prove that it is finite. Since the operator $\vartheta B\vartheta$ is bounded and self-adjoint (in view of Proposition 2.3.3)

$$\sigma(\vartheta B\vartheta) \subseteq [-\|B\|, \|B\|]. \tag{2.34}$$

Hence the sought thesis descends. ∎

Once we proved temporal boundedness of backflow for free particles, we are interested about evaluating numerically the backflow constant λ introducing the integral operator first founded by Bracken and Melloy in [6]. These authors heuristically introduce λ via time integrals of currents at point $x = 0$ over arbitrary finite intervals, motivating their definition of λ as the supremum of the spectrum of such integral operator.

2.3.8 Proposition. *Let $K : L^2(\mathbb{R}_+) \to L^2(\mathbb{R}_+)$ be the integral operator:*

$$(Kf)(u) = -\frac{1}{\pi}\int_0^\infty \frac{\sin(u^2 - v^2)}{u - v} f(v)\,\mathrm{d}v \quad \forall f \in L^2(\mathbb{R}_+). \tag{2.35}$$

Then $\vartheta B\vartheta f = Kf$ for all $f \in L^2(\mathbb{R}_+)$.

Proof. Since $\vartheta B \vartheta$ is bounded we only need to prove that $\vartheta B \vartheta = K$ holds on a dense subspace of $L^2(\mathbb{R}_+)$. Hence, we choose $\mathcal{S}(\mathbb{R}_+) := \vartheta \mathcal{S}(\mathbb{R})$, i.e. the set of Schwartz functions projected with the Heaviside function.
First of all, we relate the orthogonal projection $\mathcal{F}\vartheta\mathcal{F}^{-1}$ to the Hilbert transform

$$H : L^2(\mathbb{R}) \to L^2(\mathbb{R}), \quad (Hf)(p) = \frac{1}{\pi} PV\!\!\int_{-\infty}^{\infty} \frac{f(q)}{p-q}\, \mathrm{d}q. \tag{2.36}$$

Here PV indicates the principal value. For $f \in \mathcal{S}(\mathbb{R})$ we obtain by means of Lebesgue's dominated convergence theorem and by means of Sochozki's formula ,see [13, Example 3.3.1],

$$\begin{aligned}
(\mathcal{F}\vartheta\mathcal{F}^{-1} f)(p) &= \frac{1}{2\pi} \int_0^{\infty} e^{-ipx} \left(\int_{-\infty}^{\infty} e^{ixq} f(q)\, \mathrm{d}q \right) \mathrm{d}x \\
&= \frac{1}{2\pi} \lim_{\varepsilon \to 0^+} \int_{-\infty}^{\infty} f(q) \left(\int_0^{\infty} e^{i(q-p)x - \varepsilon x}\, \mathrm{d}x \right) \mathrm{d}q \\
&= -\frac{1}{2\pi i} \lim_{\varepsilon \to 0^+} \int_{-\infty}^{\infty} \frac{f(q)}{q-p+i\varepsilon} \mathrm{d}q \\
&= -\frac{1}{2\pi i} \left\{ PV\!\!\int_{-\infty}^{\infty} \frac{f(q)}{q-p}\, \mathrm{d}q - i\pi f(p) \right\} \\
&= \frac{1}{2i}(Hf)(p) + \frac{f(p)}{2}.
\end{aligned} \tag{2.37}$$

Hence, we have

$$\mathcal{F}\vartheta\mathcal{F}^{-1} = \frac{1}{2}(-iH + \mathbb{I}). \tag{2.38}$$

Now consider the backflow operator defined as $B = U\mathcal{F}\vartheta\mathcal{F}^{-1}U^* - U^*\mathcal{F}\vartheta\mathcal{F}^{-1}U$, where $U := \widehat{U}_{T=1}$ is the unitary evolution operator in momentum space defined in (2.17). Substituting (2.38) into the last equation, we obtain

$$B = \frac{1}{2i}(UHU^* - U^*HU). \tag{2.39}$$

From this we have for $p > 0$ and $\phi \in \mathcal{S}(\mathbb{R}_+)$

$$\begin{aligned}
(\vartheta B \vartheta \phi)(p) &= \frac{e^{-ip^2}}{2i}(HU^*\phi)(p) - \frac{e^{ip^2}}{2i}(HU\phi)(p) \\
&= \frac{1}{2\pi i} \int_0^{\infty} \frac{e^{-i(p^2-q^2)} - e^{i(p^2-q^2)}}{p-q} \phi(q)\, \mathrm{d}q \\
&= -\frac{1}{\pi} \int_0^{\infty} \frac{\sin(p^2-q^2)}{p-q} \phi(q) \mathrm{d}q = (K\phi)(p).
\end{aligned} \tag{2.40}$$

Thus the restriction of $\vartheta B \vartheta \phi$ to $L^2(\mathbb{R}_+)$ coincides with K. ∎

2.3.9 Observation. With the last proposition we proved that searching the maximum amount of backflow for any right-movers is equivalent to finding the supremum of the spectrum of a suitable integral operator. Furthermore, we have that for a generic right-mover $\psi = E_+\psi$ with $\|\psi\| = 1$

$$L(\psi_{t=0}) - L(\psi_{t=1}) = (\widehat{\psi}|K\widehat{\psi}), \tag{2.41}$$

where $L(\psi_t)$ is the probability of finding the particle in $x > 0$ at the time t, and K the operator defined in Proposition 2.3.3.

2.3.2 Maximum Backflow Approximation

As we proved in Theorem 2.3.7, there exists a lower bound for backflow. To wit, for every time interval $[0, T)$ the maximum amount of probability which could flow back for a generic right-mover is always less than $|\lambda|$. We have no information concerning λ and its eigenfunction ϕ_λ. To solve this quandary, we need to study the integral operator K. Unfortunately, no analytical value for $\sup \sigma(K)$ is known, and numerical methods have been used to estimate λ.
More precisely, we approximate $\mathbb{R}_+ \times \mathbb{R}_+$ by $[0, N\tau] \times [0, N\tau]$ divided into a grid of N^2 squares of area τ^2. In each square we approximate the kernel of the integral operator as a constant. At the same time we approximate the eigenfunction ϕ_λ as a vector φ^i_λ in $\mathbb{R}^n$ by considering the function constant in each interval $[i\tau, (i+1)\tau]$ with $i = 1, ..., n$.[1] In this way we are converting our eigenvalue-problem to a linear equation:

$$-\frac{1}{\pi}\int_0^\infty \frac{\sin(u^2 - v^2)}{u - v}\varphi(v)\,\mathrm{d}v = \lambda\varphi(u) \xmapsto{\approx} K^i_k \varphi^k_\lambda = \lambda\varphi^i_\lambda, \tag{2.42}$$

where K^i_k is the hermitian matrix obtained by approximating our integral kernel. The second equation has admits a solution. In order to find a good estimate for λ we need to take $N \to \infty$ and $\tau \to 0$. Here we report some results obtained by Braken and Melloy in their work considering $\tau = 0.05$. The estimates obtained are:

N	100	200	275	500
λ	0.0256	0.0297	0.0309	0.0323

which are apparently converging to $\lambda_{0.05} \approx 0.034$. Taking smaller values of τ and letting $N \to \infty$ we obtain the estimates $\lambda_{0.04} \approx 0.035$, $\lambda_{0.025} \approx 0.036$ and $\lambda_{0.01} \approx 0.038$.

A possible method to compute the maximum eigenvalue λ is given by Penz in [12]. It is based on an algorithm called *power iteration* and it works as follows.
Let $A \in \mathbb{C}^{N\times N}$ be a symmetric matrix and let a be the eigenvalue of A with the largest absolute value. Then, consider a vector $v_0 \in \mathbb{C}^N$ such that $v_0 \neq 0$ and there

[1] see [6, Sect. 5]

is a non-zero component within the eigenspace of A corresponding to a. Then the sequence $\{v_n\}_{n\in\mathbb{N}_0}$ recursively defined by

$$v_{n+1} = \frac{Av_n}{\|v_n\|} \tag{2.43}$$

converges to a normalized eigenvector of a. In addition, it holds[2]

$$a = \lim_{n\to\infty} v_{n+1}^{\dagger} \frac{v_n}{\|v_n\|}. \tag{2.44}$$

Since $\sigma(\vartheta B \vartheta) = \sigma(K) \subset [-1, \lambda]$, the power method can be applied to the non negative, discretized operator $\vartheta B \vartheta + \mathbb{I}$. Its largest eigenvalue then approximates $\lambda + 1$ while the sequence v_n tends to the maximizing eigenvector.
Penz started his calculations by covering a square $[0, q_0]^2$ with N_0 grid points and subsequently he repeated the computations for up to $N = N_0 h$ grid points and a larger square $[0, q]^2$ with $q = q_0\sqrt{h}$ for $h = 1, 2$, etc.. With this method, we can at the same time make the square growing and the absolute step size getting smaller. This leads to a sequence of eigenvalues λ_h as a function of the factor of accuracy h which are used to extrapolate to $h \to \infty$ and getting an approximation λ_∞ of the backflow constant. The results obtained by Penz are plotted in figure 2.3 and 2.4.

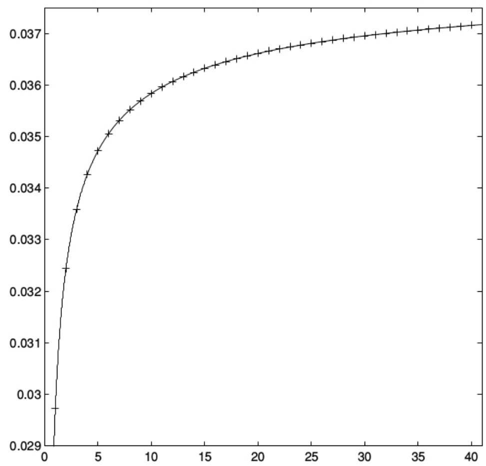

FIGURE 2.3: λ plotted against h and fit $\lambda_\infty + b/\sqrt{h}$.

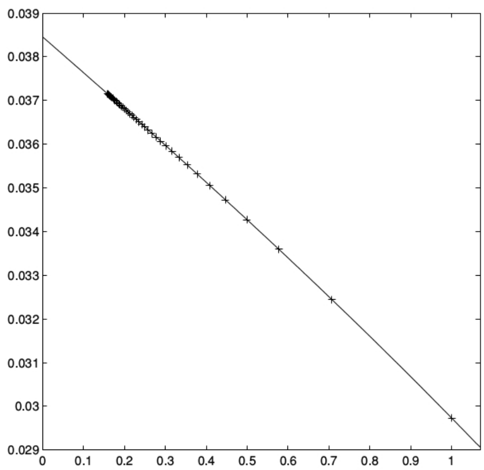

FIGURE 2.4: λ plotted against $1/\sqrt{h}$ and polynomial fit of third order.

The approximation for the backflow constant can be read off from the intersection of the y-axis with the graph in (2.4). This yields

$$\lambda \approx \lambda_\infty \approx 0.0384517. \tag{2.45}$$

[2] see [14, Sect. 7.3.1]

This is the final result computed by Penz *et al.* in [12]. Another analysis has been done by Eveson, Fewster and Verch in [8] giving an approximation for the backflow constant by $\lambda \approx 0.038452$.

Chapter 3

Interacting Quantum Backflow

The final chapter will be dedicated to the analysis of backflow in scattering theory. First of all, we shall discuss the spatial extension of backflow showing that a negative probability current might occur on arbitrary large region of space but its average value is bounded from below. After that, we extend the analysis of backflow to interacting systems, given by fairly general Hamiltonians of the form $H = P^2/2 + V(X)$, see Section 1.3.
There are two main issues concerning interacting situations:

(a) In the free case, a right-mover will preserve positive momentum for every time. In the interacting case, this is no longer true. Consider a potential which reflects the particle. The reflected wave-function entails the presence of a *classic backflow*[1] which sums up with its quantum counterpart. This is a conceptual problem since we want to study the strength of the only quantum backflow.

(b) In free theory, backflow is based on right-moving wave-function. Since in the interacting case this property is no longer preserved, we need to reformulate the problem of backflow.

In the following discussion, we will focus mainly on [7] and report their main results.

3.1 Spatially Averaged Backflow

In the last section we investigated some properties of backflow for free right-moving particles. We find out that, no matter for how long a wave function is let to evolve, the amount of probability flowing across a reference point, as per (2.11), is always larger than a dimensionless constant $-\lambda \approx 0.038$. This is a bound on the (averaged) temporal extent of backflow. Up to this, we studied backflow and the associated density probability current only at a reference point $x = 0$. We focus now the corresponding (averaged) spatial extension. In particular we want to understand

[1]Since the reflected wave goes in the opposite direction of the incident wave, this contributes negatively to the probability flux.

how negative values of j_ϕ could be distributed by considering spatial integrals of the kinematical current. In particular we will find out a lower bound similar to the one discovered in the previous section. More precisely, we will show that for all normalized right-movers ϕ and all positive averaging functions $f \geq 0$, exists $c_f \in \mathbb{R}$ such that:

$$\int_{\mathbb{R}} f(x) j_\phi(x)\,\mathrm{d}x \geq c_f > -\infty \tag{3.1}$$

Here the function f plays the role of an extended detector, generalizing the step function that we used in (2.11).
To start with, we report a result obtained in [7] concerning the possible values of the density current j_ϕ for a normalized right-moving wave function ϕ evaluated in $x = 0$.

3.1.1 Proposition (**Unboundedness of** j_ϕ)**.** *Let $x \in \mathbb{R}$. Then there exist sequences $\phi_n^\pm \in E_+(L^2(\mathbb{R}))$ of right-moving wave functions such that*

$$\lim_{n\to\infty} j_{\phi_n^\pm}(x) = \pm\infty, \tag{3.2}$$

and the norms $\|\phi_n^\pm\|_{L^2}^2$ and $\|\widehat{\phi}_n^\pm\|_{L^1}$ are independent of n.

Proof. Consider a right-moving wave function $\phi^+ \in E_+L^2(\mathbb{R})$ such that and define $\widehat{\phi}_n^+(p) := \widehat{\phi}^+(p-n)$, with $n \in \mathbb{N}$. It holds $\|\widehat{\phi}_n^+\|_{L^1} = \|\widehat{\phi}^+\|_{L^1}$ and $\|\phi_n^+\|_{L^2}^2 = \|\phi^+\|_{L^2}^2$ for all $n \in \mathbb{N}$. Furthermore, using the relation $\phi_n^+ = e^{inx}\phi^+$, and (1.38)

$$j_{\phi_n^+}(x) = j_{\phi^+}(x) + n|\phi^+(x)|^2, \tag{3.3}$$

Hence, if we choose ϕ^+ such that $\phi^+(x) \neq 0$, $\lim_{n\to\infty} j_{\phi_n^+}(x) = +\infty$. To focus in the other option, we choose a wave function χ such that $\widehat{\chi}$ has compact support on $x \in (0,\infty)$ and $\chi \neq 0$. Such function is by construction a right-mover. Now we consider the linear combinations $\widehat{\phi}_n^-(p) := \alpha_n\widehat{\chi}(p) + \beta_n\widehat{\chi}(p-n)$, where $n \in \mathbb{N}$, and $\{\alpha_n\}, \{\beta_n\} \in \mathbb{C}$ are sequences such that $|\alpha_n| = \alpha$ and $|\beta_n| = \beta$ are constant for all $n \in \mathbb{N}$. By construction, each ϕ_n^- is a right-mover and, for large n, $\|\phi_n^-\|_{L^2}^2 = (|\alpha|^2 + |\beta|^2)\|\chi\|_{L^2}^2$ while $\|\widehat{\phi}_n^-\|_{L^1} = (|\alpha| + |\beta|)\|\chi\|_{L^1}$. At this point, it only remains to choose α and β in order to have $\lim_{n\to\infty} j_{\phi_n^-}(x) = -\infty$. With this purpose, we can evaluate $j_{\phi_n^-}(x)$ obtaining:

$$j_{\phi_n^-}(x) = \begin{pmatrix}\alpha^* \\ \beta^*\end{pmatrix}^t [j_\chi(x)\mathbb{I} + nA_n] \begin{pmatrix}\alpha \\ \beta\end{pmatrix}, \tag{3.4}$$

where

$$A_n := \begin{bmatrix} 0 & e^{inx}\left(\frac{j_\chi(x)}{n} + \frac{|\chi(x)|^2}{2}\right) \\ e^{-inx}\left(\frac{j_\chi(x)}{n} + \frac{|\chi(x)|^2}{2}\right) & |\chi(x)|^2 \end{bmatrix}. \tag{3.5}$$

Here A_n is a 2×2 Hermitian matrix, whose trace is $|\chi(x)|^2$, and $\lim_{n\to\infty}\det(A_n) = -|\chi(x)|^4/4 < 0$. The eigenvalues $\lambda_\pm(n)$ of A_n converge to $\lambda_\pm(n) \to (1 \pm \sqrt{2})|\chi|^2/2$

as $n \to \infty$. Finally, choosing α_n and β_n as the coordinates of the eigenvector with the negative eigenvalue $(1-\sqrt{2})|\chi|^2/2$ (i.e. take $\alpha_n = 1/(1-\sqrt{2})$ and $\beta_n = \exp(-inx)$) we can check that $\lim_{n\to\infty} j_{\phi_n^-}(x) = -\infty$ because of the explicit factor n in front of A_n. ■

3.1.2 Observation. Before turning back to the main goal of this section, we note that the density current function j_ψ could be thought as a quadratic form defined as

$$(\psi|J(x)\psi) := j_\psi(x), \tag{3.6}$$

Here $J(x)$ could be defined as an "improper" operator (see [11]) via

$$J(x_0) = \frac{1}{2}[P\delta(X-x_0) + \delta(X-x_0)P], \tag{3.7}$$

where $\delta(X)$ is the *Dirac delta distribution.*

We can rewrite the spatially averaged density current by means of $f \in \mathcal{S}(\mathbb{R})$ as:

$$(\phi|J(f)\phi) := \int_{\mathbb{R}} f(x) j_\phi(x)\,\mathrm{d}x, \tag{3.8}$$

where $J(f)$ can be readily checked to be an (unbounded) operator, Hermitian for real f, and decomposable in terms of the position and momentum operator (X,P) as follows.

3.1.3 Definition. *Let $f \in \mathcal{S}(\mathbb{R})$. We define the* ***density current operator*** $J(f)$ *as:*

$$J(f) = \frac{1}{2}[Pf(X) + f(X)P]\,. \tag{3.9}$$

3.1.4 Remark. Note that the operator $E_+J(f)E_+$ represents the averaged current evaluated in right-moving states. The fact that backflow exists is reflected in $E_+J(f)E_+$ being non positive. To formulate this concept more rigorously we can introduce the **bottom of the spectrum** of a Hermitian operator A defined as

$$\inf(A) := \inf_{\|\phi\|=1} (\phi|A\phi) \in [-\infty, +\infty). \tag{3.10}$$

The maximal amount of backflow, spatially averaged by f, is defined as

$$\beta_0(f) := \inf(E_+J(f)E_+)\,. \tag{3.11}$$

Observe the similarities with the definition of the constant backflow λ as the infimum of a bounded and self-adjoint operator B.

Next we summarize three fundamental properties of the operator $J(f)$. The first one is the *existence* of backflow showing that $\beta_0(f) < 0$ for each positive test function f ,and more strongly *for each* function $f \neq 0$. The second property is the unboundedness of $E_+ J(f) E_+$ from above that will be proved similarly to Proposition 3.1.1. The final point regards the existence of a lower bound for our averaged current operator. In fact it will be proved that $\beta_0(f) > -\infty$, in contrast with the last Proposition where $j_\phi(x)$ has been shown to be unbounded.

3.1.5 Theorem (**Existence and boundedness of spatially averaged Backflow**). *In the context of quantum backflow, the following proposition are true:*

(a) For any $f \in \mathcal{S}(\mathbb{R})$ with $f \neq 0$, the smeared probability flow in any right-moving wave-function, $E_+ J(f) E_+$, is non positive, that is $\beta_0(f) < 0$.

(b) Let $f > 0$. Then $E_+ J(f) E_+$ is not upper bounded.

(c) Let $f > 0$. Then $E_+ J(f) E_+$, is lower bounded, i.e. $\beta_0(f) > -\infty$. Furthermore, for any test functions $f = g^2$, for $g \in \mathcal{S}(\mathbb{R})$, it holds[2]

$$\beta_0(g^2) \geq -\frac{1}{8\pi} \int_{\mathbb{R}} |g'(x)|^2 \, \mathrm{d}x > -\infty. \tag{3.12}$$

Proof. (a) First of all, we consider the operator $E_+ J(f) E_+$ and $\phi \in L^2(\mathbb{R})$. It holds

$$\begin{aligned} &\mathcal{F} E_+ J(f) E_+ \phi = \mathcal{F} E_+ J(f) \mathcal{F}^{-1} \mathcal{F} E_+ \phi = \vartheta(q) \mathcal{F} J(f) \mathcal{F}^{-1} \vartheta(p) \widehat{\phi}(p) = \\ &= \frac{1}{2} \mathcal{F} f(x) \mathcal{F}^{-1} (p+q) \vartheta(q) \vartheta(p) \widehat{\phi}(p) = \int_{-\infty}^{\infty} \mathrm{d}p \, \frac{p+q}{2\sqrt{2\pi}} \widehat{f}(q-p) \vartheta(p) \vartheta(q) \widehat{\phi}(p). \end{aligned} \tag{3.13}$$

Hence we have identified the integral kernel

$$K_f(q,p) = \frac{p+q}{2\sqrt{2\pi}} \widehat{f}(q-p) \vartheta(p) \vartheta(q), \tag{3.14}$$

Taking the restriction of K_f to $L^2(\mathbb{R}_+, \mathrm{d}p)$, we can neglect the Heaviside functions. We shall prove non-positivity of $E_+ J(f) E_+$ by contradiction. Hence, suppose $E_+ J(f) E_+$ were positive. Then,

$$\int_0^{+\infty} \mathrm{d}q \int_0^{+\infty} \mathrm{d}p \, \varphi^*(q) K_f(q,p) \varphi(p) > 0 \ \forall \varphi \in L^2(\mathbb{R}_+, \mathrm{d}p)\,. \tag{3.15}$$

Consider a sequence $\{g_n\} \in L^2_0(\mathbb{R})$ of functions converging to the Dirac delta distribution δ_0, and $\alpha, \beta \in \mathbb{C}$. It holds

$$\begin{aligned} \int_0^{+\infty} \mathrm{d}q' \int_0^{+\infty} \mathrm{d}p' \, [\alpha^* g_n^*(q'-q) + \beta^* g_n^*(q'-p)] K_f(q',p') \times \\ \times [\alpha g_n(q'-q) + \beta g_n(q'-p)] > 0, \end{aligned} \tag{3.16}$$

[2] see [8]

for all $n \in \mathbb{N}$, $\alpha, \beta \in \mathbb{C}$, and $p, q > 0$. So, taking the limit $n \to \infty$,

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix}^{\dagger}\begin{bmatrix}K_f(q,q) & K_f(q,p)\\ K_f(q,p) & K_f(p,p)\end{bmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} > 0 \; \forall \alpha, \beta \in \mathbb{C}, \; \forall p, q > 0. \tag{3.17}$$

In this paragraph we have proved $E_+ J(f) E_+$ is positive if so is the Hermitian 2×2 matrix (3.17) for each choice of $p, q > 0$. This amounts to the matrix must having only non-negative eigenvalues, which in turn is implemented by a non-negative determinant and trace. The former reads

$$0 \leq K_f(q,q)K_f(p,p) - |K_f(q,p)|^2 = \frac{pq}{2\pi}|\widehat{f}(0)|^2 - \frac{(p+q)^2}{8\pi}|\widehat{f}(q-p)|^2 \tag{3.18}$$

i.e.

$$|\widehat{f}(q-p)| \leq \frac{2\sqrt{pq}}{p+q}|\widehat{f}(0)|. \tag{3.19}$$

Now we can show that, taking $q \to 0$ at fixed $p > 0$, $|\widehat{f}(-p)| = 0$ for all $p > 0$. Yet, since f is real, $\widehat{f}(-p) = \widehat{f}^*(p)$, so that $\widehat{f}(p) = 0$ for each $p \neq 0$. As the test function f is continuous, this implies that f vanishes altogether. So we conclude that for any real $f \neq 0$ the operator $E_+ J(f) E_+$ is not positive.
(b) The proof of this point is pretty similar to the one of Proposition 3.1.1. In fact, consider a normalized right-moving function $\phi = E_+\phi \in L^2(\mathbb{R})$, and define a sequence of shifted-momentum wave functions $\widehat{\phi}_n(p) = \widehat{\phi}(p-n)$ with $n \in \mathbb{N}$. It holds that $\|\phi_n\|_{L^2} = 1$ and $E_+\phi_n = \phi_n$. Furthermore, the expectation value of $E_+ J(f) E_+$ is

$$(\phi_n|E_+ J(f) E_+ \phi_n) = (\phi|E_+ J(f) E_+ \phi) + n\int_{-\infty}^{+\infty} f(x)|\phi(x)|^2 \,\mathrm{d}x. \tag{3.20}$$

For $f > 0$, it is clear that there exists ϕ such that the last integral is positive and in this case we have $\lim_{n\to\infty}(\phi_n|E_+ J(f) E_+ \phi_n) = +\infty$, showing that the operator $E_+ J(f) E_+$ has no finite upper bound.
(c) In order to prove the final statement of this theorem, we consider a general normalized right-moving function $\phi = E_+\phi \in L^2(\mathbb{R})$ and $g \in \mathcal{S}(\mathbb{R})$. The averaged spaced density current reads

$$\begin{aligned}(\phi|E_+ J(g^2) E_+) &= Re(\phi|g^2(X)P\phi)\\ &= Re[(\phi|g(X)Pg(X)\phi) + (\phi|g(X)[g(X),P]\phi)]\\ &= Re[(\phi|g(X)Pg(X)\phi) + i(\phi|g(X)g'(X)\phi)]\\ &= Re(\phi|g(X)Pg(X)\phi) = (g(X)\phi|Pg(X)\phi)\\ &= \int_{-\infty}^{+\infty} p|\mathcal{F}[g(X)\phi](p)|^2 \,\mathrm{d}p.\end{aligned} \tag{3.21}$$

Here $[g(X), P]$ is equal to $ig'(X)$. Considering the integral only on $(-\infty, 0)$, we obtain:

$$(\phi|E_+ J(g^2) E_+ \phi) \geq \int_{-\infty}^{0} p|\mathcal{F}[g(X)\phi](p)|^2 \,\mathrm{d}p = -\int_{0}^{\infty} p|\mathcal{F}[g(X)\phi](-p)|^2 \,\mathrm{d}p. \tag{3.22}$$

By the Convolution Theorem 1.2.12 we can rewrite $\mathcal{F}[g(X)\phi]$ as

$$\mathcal{F}[g(X)\phi](p) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \mathrm{d}p' \, \widehat{\phi}(p')\widehat{g}(p-p'), \tag{3.23}$$

where the restriction to $p' > 0$ is a consequence $E_+\phi = \phi$. Now, applying the Cauchy-Schwarz theorem, we obtain:

$$\begin{aligned} |\mathcal{F}[g(X)\phi](-p)|^2 &= \left| \frac{1}{\sqrt{2\pi}} \int_0^\infty \mathrm{d}p' \, \widehat{\phi}(p')\widehat{g}(-p-p') \right|^2 \\ &\leq \frac{\|\phi\|^2}{2\pi} \int_0^\infty \mathrm{d}p' \, |\widehat{g}(-p-p')|^2 = \frac{1}{2\pi} \int_0^\infty \mathrm{d}p' \, |\widehat{g}(p+p')|^2, \end{aligned} \tag{3.24}$$

where we have also used $|\widehat{g}(-p)|^2 = |\widehat{g}(p)|^2$ (being g real valued) and $\|\phi\| = 1$. Substituting into (3.22),

$$\begin{aligned} (\phi|E_+J(g^2)E_+\phi) &\geq -\frac{1}{2\pi} \int_0^\infty \mathrm{d}p \int_0^\infty \mathrm{d}p' \, p|\widehat{g}(p+p')|^2 \\ &= -\frac{1}{2\pi} \int_0^\infty \mathrm{d}u \, |\widehat{g}(u)|^2 \int_0^u \mathrm{d}p \, p \\ &= -\frac{1}{4\pi} \int_0^\infty \mathrm{d}u \, u^2 |\widehat{g}(u)|^2 \\ &= -\frac{1}{8\pi} \int_{-\infty}^\infty \mathrm{d}u \, u^2 |\widehat{g}(u)|^2 \\ &= -\frac{1}{8\pi} \int_{-\infty}^\infty \mathrm{d}x \, |g'(x)|^2 \ \forall \phi \in L^2(\mathbb{R}), \end{aligned} \tag{3.25}$$

where we have changed the variables (p, p') to (u, p) with $u = p + p'$. We enjoyed that $|\widehat{g}(u)|^2$ is even as well as and Parseval's theorem . This last equation complete the proof of the inequality (3.12). This also proves the boundedness of $E_+J(f)E_+$ for all Schwarz functions $f > 0$ since there always exists $g \in \mathcal{S}(\mathbb{R})$ such that $g^2 = f$. ■

Until now, we considered right-moving functions at a fixed time and no assumption on any potentials has been made so far. In the following section we start the analysis of backflow in scattering theory by introducing the concept of *interacting state* and *asymptotic solutions* of Schrödinger equation.

3.2 Backflow and Scattering

Let us consider a physical system described by an Hamiltonian $H = \frac{1}{2}P^2 + V(X)$, where $V(X)$ is a general time-independent potential described as a function of the position X. We wonder whether backflow could occur and if there exists a lower bound for the averaged spatial density current. The first conceptual problem that we encounter is that in non-zero potential situation, the space of right-movers $E_+(L^2(\mathbb{R}))$ is no longer invariant under time evolution. Hence, it is more difficult to define when a particle "travels to the right"[3]. To overcome this, we can substitute the concept of right-moving solutions with the "asymptotic momentum" distributions in the sense of scattering theory. Heuristically, we consider solutions such that for $t \to -\infty$ the associated wave-function is a right-mover in the usual sense. This space has the property to be invariant under time evolution and describes particles scattering "from the left" into the potential wall. The link between an asymptotic, free state ψ and the interacting counterpart is ruled by the *Møller operator*:

$$\Omega_V := \lim_{t \to -\infty} e^{iHt} e^{-iH_0 t}, \tag{3.26}$$

where H_0 is the free Hamiltonian $P^2/2$. As mentioned in Chapter 1 the last equation has to be read in this way[4]: Consider a particle which scatters against a potential wall V at the time $t = 0$. Its dynamics is described by Schrödinger equation

$$i\partial_t \psi(t) = H\psi(t), \quad \psi(0) = \psi_0\,, \tag{3.27}$$

Until the particle is sufficiently distant from the potential wall, it behaves like a free particle. Stated differently, we state that $\psi(t)$ has "free" asymptotics as $t \to -\infty$ if there exists $u_0 \in L^2(\mathbb{R})$ such that

$$\lim_{t \to -\infty} \|\psi(t) - u(t)\| = 0, \quad u(t) := \exp(-iH_0 t) u_0\,. \tag{3.28}$$

Relation (3.28) leads to a connection between the corresponding initial data ψ_0 and u_0,

$$\psi_0 = \lim_{t \to -\infty} e^{iHt} e^{-iH_0 t} u_0 = \Omega_V u_0. \tag{3.29}$$

3.2.1 Observation. Observe that, although Ω_V is not unitary in the presence of bound states, we still have $\|\Omega_V\| = 1$.

We focus on the averaged probability current $J(f)$ in an asymptotically right-moving state.

3.2.2 Definition. *Let $J(f)$ be the density current operator defined in (3.9), and let E_+ be the orthogonal projector on the space of right-movers. Let Ω_V be the Møller operator. We call $E_+\Omega_V^* J(f)\Omega_V E_+$. the* ***asymptotic current operator***

3.2.3 Remark. The goal of this section is to investigate the spectral properties of this operator, and how to estimate the *backflow constant*:

$$\beta_V(f) := \inf(E_+\Omega_V^* J(f)\Omega_V E_+). \tag{3.30}$$

[3] see [7, Sect. III]
[4] see [16, Chapt. 0, Sect. 4]

For scattering theory to be well defined, we need to impose our potentials $V(x)$ to be sufficiently rapidly decreasing as $x \to \pm\infty$.

3.2.4 Definition. *We define $L^{1+}(\mathbb{R})$ the set of all real functions V such that the norm*

$$\|V\|_{1+} := \int_{-\infty}^{\infty} (1+|x|)|V(x)| \,\mathrm{d}x < \infty \tag{3.31}$$

exists finite.

3.2.5 Observation. Let $V \in L^{1+}$, the time-independent Schrödinger equation for scattering states reads:

$$[-\partial_x^2 + 2V(x) - k^2]\psi(x) = 0 \;\; k \in \mathbb{R}. \tag{3.32}$$

In the stationary picture of scattering theory, we seek solutions φ_k, $k > 0$, of (3.32) with the following asymptotics:

$$\varphi_k(x) = \begin{cases} T_V(k)e^{ikx} + o(1) & \text{for } x \to +\infty \\ e^{ikx} + R_V(k)e^{-ikx} + o(1) & \text{for } x \to -\infty \end{cases} \tag{3.33}$$

where $R_V(k)$ and $T_V(k)$ denote the reflection and transmission coefficients of the potential V, respectively, and are uniquely determined by V. In other words we choose all those solutions behaving like plane waves which scatter against a potential wall, resulting into a transmitted plane wave $e^{ikx}T_V(k)$ and into a reflected one $R_V(k)e^{-ikx}$ (See Fig. (3.2)).

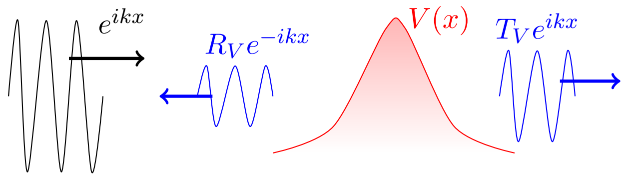

FIGURE 3.1: Sketch of a scattering process of a plane wave with momentum k into a potential $V(x)$ resulting into reflected and transmitted waves as Eq. (3.33)

At this point, we shall recall a few results of scattering theory. A deeper and more exhaustive analysis of the mathematical aspects of scattering theory could be found in [16].

3.2.6 Lemma. *Let $V \in L^{1+}(\mathbb{R})$. Then the Møller operator Ω_V exists. Furthermore, the solution $x \mapsto \varphi_k(x)$ $(k > 0)$ of (3.32) with the asymptotic conditions (3.33) exists and it is unique. In addition, for any $\widehat{\psi} \in C_0^\infty(\mathbb{R})$,*

$$(\Omega_V E_+ \psi)(x) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \varphi_k(x)\widehat{\psi}(k)\,\mathrm{d}k. \tag{3.34}$$

We will stick to report the references where finding an exhaustive proof of this lemma. Existence and uniqueness of solution φ_k are a consequence of [16, Chap. 5, Lemma 1.1]. Existence of Ω_V, under milder assumptions on V, can be found in [16, Chap. 5, Theorem 1.12].

3.2.7 Observation. Let us dwell further on the meaning of Eq. (3.34). We are considering a smooth wave-function ψ with momentum representation $\widehat{\psi} \in C_0^\infty(\mathbb{R})$, though we are interested only in "right-moving" solutions. Then, we will not consider the function $\widehat{\psi}(k)$ for $k < 0$. Considering only the "right-moving" components of ψ we can think of it as the sum of plane wave-functions $e^{ikx}\widehat{\psi}(k)$ (parametrized in $k > 0$) which scatter into the potential V giving the solutions φ_k. The integral of all this scattered components will give the solution $\Omega_V E_+ \psi$.

3.2.8 Remark. From here on, we will consider only wave-functions ψ such that $\widehat{\psi} \in C_0^\infty(\mathbb{R})$ as in Lemma 3.2.6 in order to have a well defined asymptotic current operator $E_+\Omega_V^* J(f)\Omega_V E_+$.

3.2.9 Observation. Using (3.34), we are able to estimate the expectation values of the asymptotic current operator as follows

$$(\psi|E_+\Omega_V^* J(f)\Omega_V E_+\psi) = \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \int_0^\infty \mathrm{d}p \int_0^\infty \mathrm{d}q\, \widehat{\psi}^*(p) K_V(p,q,x)\widehat{\psi}(q), \tag{3.35}$$

where K_V is

$$K_V(p,q,x) = \frac{i}{4\pi}[\partial_x \varphi_p^*(x)\varphi_q(x) - \varphi_p^*(x)\partial_x\varphi_q(x)]. \tag{3.36}$$

Following [7], the next step in our analysis is to establish bounds on the solution φ_k and K_V relating them to their spatial asymptotics. As in the previous lemma, we will not give any proof, but only pointing to relevant references.

3.2.10 Lemma. *Let $V \in L^{1+}(\mathbb{R})$ and let φ_k, with $k > 0$, be the solution of (3.32) with the asymptotics (3.33). Let K_V be as in (3.36). Then, there exist constants $c_V, c_V', c_V'', c_V''' > 0$ such that for all $x \in \mathbb{R}$ and $p, q, k > 0$*

$$|\varphi_k(x)| \le c_V(1 + |x|), \tag{3.37}$$

$$|\varphi_k(x)e^{ikx}| \le c_V' \frac{1+|x|}{1+k}, \tag{3.38}$$

$$|\partial_x\varphi_k(x) - ik\varphi_k(x)| \le c_V'' \frac{1}{1+k}, \tag{3.39}$$

$$\left| K_V(p,q,x) - \frac{p+q}{4\pi}\varphi_p^*(x)\varphi_q(x) \right| \le c_V'''(1+|x|). \tag{3.40}$$

The first two bounds in (3.37) and (3.38) can be deduced from [17, Sec. 2, Lemma 1], paying attention to the fact that the function $m(x, k)$ there corresponds to our

$\varphi_k(x)e^{-ikx}/T_V(k)$, while $T_V(k)$ is such that $|T_V(k)| \leq 1$ and $T_V(k) = 1 + O(1/k)$ for large k [17, Sec. 2, Theorem 1]. The last two bounds in (3.39) and (3.40), are consequence of (3.37) and (3.38). The constants c_V, c'_V, c''_V, and c'''_V can be deduced from [17] as functions of V, although they are not optimal and we will not use them during the following discussion.
With this information in mind, we have arrived to the first main result for backflow in scattering theory. We will prove the unboundedness of the asymptotic current operator $E_+\Omega_V^* J(f)\Omega_V E_+$ and the existence of backflow as well as the presence of negative parts of the spectrum, generalizing the results of the free situation, see Th. 3.1.5.

3.2.11 Theorem (Existence of backflow in scattering situations). *Let $V \in L^{1+}(\mathbb{R})$. Then,*

(a) for every $f \in \mathcal{S}(\mathbb{R})$ with $f > 0$, there is no finite upper bound on the asymptotic current operator $E_+\Omega_V^* J(f)\Omega_V E_+$,

(b) for every $x \in \mathbb{R}$, there is a sequence of normalized right-movers $\psi_n = E_+\psi_n$ such that $\lim_{n\to\infty}(\psi_n|\Omega_V^* J(x)\Omega_V\psi_n) = -\infty$.

3.2.12 Observation. Before proving Theorem 3.2.11, let us note that point (b) means that the backflow constant $\beta_V(f)$ could be negative for some positive f. Thus, averaged backflow exists in all scattering situations. The difference with the free case is that $\beta_0(f)$ ought to be negative for all positive Schwarz functions f, see Th. 3.2.11 In scattering scenarios, we are not able to give an analogous statement for $\beta_V(f)$.

Proof of Theorem 3.2.11. (a). To prove unboundedness of $E_+\Omega_V^* J(f)\Omega_V E_+$, we recall what done in Theorem 3.1.5 (b). Hence, we consider a right-mover $\psi = E_+\psi$ such that $\widehat{\psi} \in C_0^\infty(\mathbb{R}_+)$ and shift it to higher momenta defining the sequence $\widehat{\psi}_n(p) := \widehat{\psi}(p-n)$. In view of the unboundedness of $(\psi_n|E_+J(f)E_+\psi_n)$ from above [as in Theorem 3.1.5(b)], we only need to show that the sequence $(\psi_n|(\Omega_V^* J(f)\Omega_V - J(f))\psi_n)$ is bounded as $n \to \infty$. In fact, from (3.35) it holds

$$\begin{aligned}(\psi_n|(\Omega_V^* J(f)\Omega_V - J(f))\psi_n) = \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \int_{\mathbb{R}_+^2} \mathrm{d}p\, \mathrm{d}q \,\times \\ \times \left\{ \widehat{\psi}_n^*(p)\widehat{\psi}_n(q) \left[K_V(p,q,x) - \frac{p+q}{4\pi}\varphi_p^*(x)\varphi_q(x) \right] + \right. \\ \left. + \widehat{\psi}^*(p)\widehat{\psi}(q)\frac{p+q+2n}{4\pi}\left[\varphi_{p+n}^*(x)\varphi_{q+n}(x) - e^{i(q-p)x}\right] \right\}, \end{aligned} \tag{3.41}$$

where φ are the solutions taken from Lemma 3.2.6. Since the norms $\|\widehat{\psi}_n\|_{L^1}$ are independent from n, the first integrand is bounded in view of (3.40). (3.37) and (3.38) yield the same for the second integrand. This proves point (a).
(b) Non-positivity of the asymptotic current operator $E_+\Omega_V^* J(f)\Omega_V E_+$ could be

proved similarly. Here we take a sequence of right-movers ψ_n^- as in Proposition 3.1.1. Then, it suffices to show that $(\psi_n|(\Omega_V^* J(f)\Omega_V - J(x))\psi_n)$ is bounded in the same way as in point (a), using a suitable choice of χ, such that $\widehat{\chi} \in C_0^\infty(\mathbb{R}_+))$ as in Proposition 3.1.1. ■

Now, we are ready for the main result of this chapter: the boundedness of the backflow constant $\beta_V(f)$ for every fixed non-negative $f \in \mathcal{S}(\mathbb{R})$, with potential $V \in L^{1+}(\mathbb{R})$. For this purpose, we need to take the asymptotic current operator $E_+\Omega_V^* J(f)\Omega_V E_+$ and split it into several terms (see in Observation (3.2.14)).

3.2.13 Observation. Consider the projector into the "left-movers" space E_- from Definition 2.2.3 and let the operator T_V act by multiplication with the transmission coefficient $T_v(k)$ from (3.33) in momentum space. Hence, it holds true that

(i) T_V commutes with $E_\pm$ and $E_-T_VE_+ = E_-E_+T_V = 0$. The first statement descends from $E_\pm$ anf T_V being defined as multiplicative operators in momentum space and the second from the identity $E_\pm E_\mp = 0$.

(ii) $E_-\Omega_V E_+ = E_-(\Omega_V - T_V)E_+$ as consequence of point (i).

3.2.14 Observation (Bounds of current operator). Via the identities $E_- + E_+ = \mathbb{I}$ and $(i+P)^{-1}(i+P) = \mathbb{I}$, it holds

$$\begin{aligned}
E_+\Omega_V^* J(f)\Omega_V E_+ &= E_+\Omega_V^*(E_- + E_+)J(f)(E_- + E_+)\Omega_V E_+ \\
&= E_+\Omega_V^* E_+ J(f) E_+ \Omega_V E_+ \\
&+ E_+\Omega_V^* E_+ J(f)(i+P)^{-1}E_-(i+P)(\Omega_V - T_V)E_+ \\
&+ E_+(\Omega_V^* - T_V^*)(-i+P)E_-(-i+P)^{-1}J(f)\Omega_V E_+.
\end{aligned} \tag{3.42}$$

Here we used the results from Observation 3.2.13, the commutativity between $(i+P)$ and $E_\pm$ and $(i+P)^* = (-i+P)$. Note that the first term on the right side of (3.42) is bounded by the constant $\beta_0(f)$, as proved in Theorem 3.1.5, and $\|E_+\| = \|\Omega_V\| = 1$. We must evaluate the other terms on the right hand side of (3.42) in order to prove the existence of maximum backflow. In particular we want to show that

$$\begin{aligned}
\inf(E_+\Omega_V^* J(f)\Omega_V E_+) &\geq \beta_0(f) - 2\|J(f)(i+P)^{-1}\|\|(i+P)(\Omega_V - T_V)E_+\| \\
&\geq \beta_0(f) - 2\|J(f)(i+P)^{-1}\|[2 + \|P(\Omega_V - T_V)E_+\|],
\end{aligned} \tag{3.43}$$

where the norms $\|J(f)(i+P)^{-1}\|$ and $\|P(\Omega_V - T_V)E_+\|$ ought to be finite.

In order to estimate $\|J(f)(i+P)^{-1}\|$, it is useful to introduce the concept of Green's distribution. The Green distribution, or fundamental solution, of a linear differential operator L is the distribution G such that $LG = \delta$, where δ is the Dirac's delta distribution[5]. In our case, we are interested in finding the Green's function of the time-independent Schrödinger equation (3.32).

[5]see [2, Chapt. 5, Sect. 3-4]

3.2.15 Proposition. *Consider the function $G_k(x)$ defined as*

$$G_k(x) := \frac{\sin(kx)}{k}\vartheta(x). \tag{3.44}$$

Then, G_k is the solution of equation $-G_k''(x) = k^2 G_k(x) - \delta(x)$ in the sense of distributions, i.e. G_k is the fundamental solution of the time-independent Schrödinger equation (3.32).

The solution φ_k of (3.32) could be uniquely determined using G_k via the following integral equation (Lippman-Schwinger equation)

$$\varphi_k(x) = T_V(k)e^{ikx} + \int_{-\infty}^{\infty} 2V(y)G_k(y-x)\varphi_k(y)\,\mathrm{d}y, \tag{3.45}$$

where (3.45) is the convolution between G_k and $\varphi_k \cdot V$. With this information at hand,

3.2.16 Proposition. *Let $V \in L^{1+}(\mathbb{R})$. Then*

$$\|P(\Omega_V - T_V)E_+\| \leq 2c_V\|V\|_{1+}\,, \tag{3.46}$$

with the constant c_V being the one in Lemma 3.2.10.

Proof. Consider ξ, ψ such that $\widehat{\xi}, \widehat{\psi} \in C_0^\infty(\mathbb{R})$ and $\psi = E_+\psi$. Lemma 3.2.6 yields

$$\begin{aligned}(\xi|P(\Omega_V - T_V)\psi) &= (P\xi|(\Omega_V - T_V)\psi) \\ &= \frac{i}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}x\,\xi'^*(x)\int_0^\infty \mathrm{d}k\,[\varphi_k(x) - T_V(k)e^{ikx}]\widehat{\psi}(k).\end{aligned} \tag{3.47}$$

The expression above may be rewritten in view of (3.45), using Fubini's theorem and integration by parts. Thus, we obtain

$$\begin{aligned}(\xi|P(\Omega_V - T_V)\psi) &= \frac{i}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}x\,\xi'^*(x)\int_0^\infty\mathrm{d}k\int_{-\infty}^{\infty}\mathrm{d}y\,2V(y)G_k(y-x)\varphi_k(y). \\ &= \frac{2i}{\sqrt{2\pi}}\int_{\mathbb{R}^2}\mathrm{d}x\,\mathrm{d}y\int_0^\infty\mathrm{d}k\,\xi(x)^*V(y)\cos[k(y-x)]\vartheta(y-x)\varphi_k(y)\widehat{\psi}(k)\end{aligned} \tag{3.48}$$

Consider the multiplicative operator M_y, with $y \in \mathbb{R}$, defined as

$$(M_y\psi)(k) := \mathcal{F}^{-1}[\varphi_k(y)\widehat{\psi}(k)] \tag{3.49}$$

and the integral operator I_y

$$(I_y\widehat{\psi})(x) := \vartheta(y-x)\int_0^\infty \cos[k(y-x)]\widehat{\psi}(k)\,\mathrm{d}k. \tag{3.50}$$

As noted in [7, Prop. 2], $\|I_y\| \leq \sqrt{2\pi}$ for all $y \in \mathbb{R}$. Using Lemma 3.2.10 and (3.37), we establish the following bound for M_y:

$$\|M_y\psi\| \leq (c_V(1+|y|))\|\psi\| \Rightarrow \|M_y\| \leq c_V(1+|y|) \; \forall y \in \mathbb{R}. \tag{3.51}$$

Replacing the previous bounds in (3.48), yields

$$\begin{aligned} |(\xi|P(\Omega_V - T_V)\psi)| &\leq \frac{2\|\xi\|\|\psi\|}{\sqrt{2\pi}} \int_{-\infty}^{\infty} |V(y)|\|I_y\|\|M_y\| \, \mathrm{d}y \\ &\leq 2c_V\|\xi\|\|\psi\| \int_{-\infty}^{\infty} |V(y)|(1+|y|) \, \mathrm{d}y \\ &\leq 2c_V\|V_y\|_{1+}\|\xi\|\|\psi\|. \end{aligned} \tag{3.52}$$

Since ξ and ψ are taken respectively from a dense subspace of $L^2(\mathbb{R})$ and $E_+L^2(\mathbb{R})$, this concludes the proof. ■

Summing up all results obtained in Observation 3.2.14, (3.42), and Proposition 3.2.16, it holds the following[6]

3.2.17 Theorem (Boundedness of backflow in scattering situations). *For any potential $V \in L^{1+}(\mathbb{R})$ and for any non-negative $f \in \mathcal{S}(\mathbb{R})$, there exists a lower bound on the spatially averaged backflow:*

$$\beta_V(f) \geq \beta_0(f) - [2\|f\|_\infty + \|f'\|_\infty](2 + 2c_V\|V\|_{1+}) > -\infty, \tag{3.53}$$

where $\|f\|_\infty := \sup_{x\in\mathbb{R}} |f(x)|$, $\beta_0(f)$ is the backflow constant in Th. 3.1.5, and c_V is the constant from Lemma 3.2.10.

Proof. To prove this bound we reconsider (3.43)

$$\inf(E_+\Omega_V^* J(f)\Omega_V E_+) \geq \beta_0(f) - 2\|J(f)(i+P)^{-1}\|[2 + \|P(\Omega_V - T_V)E_+\|]. \tag{3.54}$$

Following Observation 3.2.14, we must prove the existence of a bound for $\|P(\Omega_V - T_V)E_+\|$ and $\|J(f)(i+P)^{-1}\|$. The first one is given by Proposition 3.2.16. To prove that for $\|J(f)(i+P)^{-1}\|$, we note from the definition of $J(f)$ in (3.9) that

$$J(f) = \frac{1}{2}[Pf(X) + f(X)P] = \frac{1}{2}\Big[[P, f(X)] + 2f(X)P\Big] = f(X)P - \frac{i}{2}f'(X). \tag{3.55}$$

Hence we have $\|J(f)(i+P)^{-1}\| \leq \|f\|_\infty + \frac{1}{2}\|f'\|_\infty$. Replacing everything in (3.54), the thesis follows. ■

The last theorem concludes our investigation on the existence of backflow in an interacting scenario. We have shown that the asymptotic current operator

[6] see [7, Th. 3]

$E_+\Omega_V^* J(f)\Omega_V E_+$ is bounded from below. Thus, in any scattering scenario backflow can occur, but its value spatially averaged under a non-negative test-function f is always bigger than the constant $\beta_V(f)$. Note that (3.53) says very little about the actual value of this bound and a numerical analysis is needed for different types of potentials V. Some examples are given in [7, Sect. IV].

Conclusions

In this thesis we described the quantum-mechanical phenomenon of *backflow* in the non-interacting and interacting scenario, using methods from operator theory. In particular, we outlined the fundamental properties of backflow effect and its strength in different frameworks.
In Chapter 2, we ~~formulate rigorously the definition~~ of backflow for free particles ~~via~~ introducing the concept of *right-movers* as those wave-function with only positive momenta. ~~We proved that backflow can occur via showing some examples of right-moving wave functions in which the density probability current points backwards~~. Then, we investigated the flux of probability through a reference point during a given interval of time and for a given normalized right-mover. We showed that the lower bound in the amount of probability which might "flow backwards" is equivalent to the infimum of the spectrum of a suitable operator B, called *backflow operator*. We proved that B is bounded and self-adjoint and hence that ~~this lower bound λ exists, called the *backflow constant*~~. ~~We described the *power method* in order to evaluate an approximation for λ, obtaining $\lambda \approx 0.038452$.~~
In Chapter 3, we generalized these results ~~for~~ interacting scenarios. In particular, we considered particles scattering ~~against some~~ short-range potential V and investigated the existence of backflow in this framework. ~~We needed to~~ reformulate the problem of backflow by defining *asymptotic right-movers*, as those wave-functions that ~~far in the past~~ ~~were behaving~~ like free right-movers, ~~and by introducing some basic concept from scattering theory such the *Møller operator* Ω_V~~. Then we analyzed the spatially averaged current

$$\int_{-\infty}^{\infty} f(x) j_{\Omega_V \psi}(x)\,\mathrm{d}x\,,$$

with $\Omega_V \psi$ represents the wave-function of an interacting particle, ~~and wonder whether this integral might assume negative values or not for all smearing positive functions $f \geq 0$.~~ As in chapter 2, we needed to evaluate the infimum of the spectrum of a proper operator, called *asymptotic current operator.* In the end, we proved that such operator is bounded from below ~~and hence that~~, for each short-range potential V and smearing positive function $f \geq 0$, there exists a constant $\beta_V(f) \in (-\infty, 0)$ such that the spatially averaged backflow is always larger than $\beta_V(f)$. The existence of backflow might seem not surprising for potentials with reflection, because reflection processes clearly produce probability flow to the left. But our results also holds for reflection-less potentials, ~~in which backflow exists, but turns out to be weaker than in the free case~~[7].

The possible extensions and follow-ups of this work are many. Firstly, numerical methods can be used to estimate the constant $\beta_V(f)$ for different averaging functions f and potential V. In [7, Sect. IV], this analysis is made by considering Gaussian function for f and *Delta potential* $V(x) = \alpha\delta(x)$ as well as the reflection-less *Pöschl-Teller potential*

$$V(x) = -\frac{\mu(\mu+1)}{2\cosh^2(x)} \quad \text{with } \mu \in \mathbb{N}\,.$$

Secondly, we remark that backflow has been studied only theoretically and no experimental observations were been conducted. The weakness of backflow represents a remarkably issue for any experimental set-up that try to measure this quantum effect. A possible experimental scheme that could lead to the first observation of quantum backflow is made by Palmero *et al.* in [9]. They proposed to use Bose-Einstein condensates. In detail, ~~following their discussion~~, the application of a positive momentum kick, via a Bragg pulse[8], to such a condensate with a positive velocity may cause a current flow in the negative direction. A sketch of the experimental set-up, as in Figure 3.2, is the following:

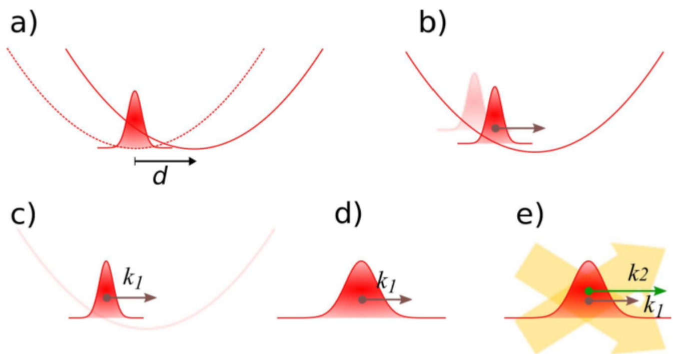

FIGURE 3.2: Sketch of the experimental set-up proposed in [9]

(a) A condensate is created in the ground state of a harmonic trap with frequency ω ; at $t = 0$ a magnetic gradient is applied, shifting the trap by a distance d.

(b) The condensate starts to perform dipole oscillations in the trap.

(c) When the condensate reaches a desired momentum k_1, the trap is switched off.

[7] see [7, Sect. I]

[8] For a more detailed discussion on the Bragg pulse, see [18]

(d) The condensate is let to expand for a time t.

(e) Finally, a Bragg pulse is applied in order to transfer part of the ~~to a~~ state of momentum k_2. The superposition of state with momentum k_1 and $k_2 > k_1$~~, as well as in the examples in Section 2.2, may cause backflow.~~

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